Abram I. Fet

Group Theory of Chemical Elements

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Structure and Properties of Elements and Compounds

DE GRUYTER


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Contents

Preface to the English edition

It is well known that multi-electron Schrödinger equation can give only approximate solutions. Empirical and semi-empirical methods used to find them are not accurate and hence they describe the properties and behavior of chemical elements only approximately. The author of this book applied group-theoretical approach, which proved to be effective in building the system of hadrons, to describe qualitatively the properties of chemical compounds which cannot be derived from the equations. This is the main result of his work.

This book is useful in yet another respect. It makes the theory accessible to the reading audience with a general chemical background. The author starts with common, familiar subjects and introduces further the ideas of the physics of symmetry as naturally as possible, so that its origin and meaning can be understood without profound background in mathematical apparatus of quantum physics.

This book is in no way purely theoretical. Rather, it has strong connections with experimentally measured properties of chemical elements and their compounds. To compare the theory with experiments, the author considered the properties of elements that are associated with their chemical behavior: ionization potentials, atomic volumes, enthalpies of formation of the elements, polarizability of the atoms, their boiling and melting points, enthalpy of vaporization, electron affinity, energies of ionic lattices, and bonding energies of diatomic molecules and some lanthanide compounds.

The obtained confirmations of the theory suggested that it would be useful to understand the properties of chemical compounds. These hopes largely justified. This book can be regarded a generalization of the ideas presented in the existing literature on this subject.

I express my deep gratitude to my colleagues from different countries whose judgements strengthened my intention to publish the book in English.

Rem Khlebopros

Introduction

This book presents a group description of chemical elements considered as states of a quantum system. Atoms of different elements are viewed as elements of a vector space associated with an irreducible unitary representation of some symmetry group. The elements of the group are carried into each other by operators defined on this group. This approach fundamentally differs from the traditional application of group theory to atomic physics, where a symmetry group is used to carry into each other different excited states of the same atom. Besides, we describe heavy particles (hadrons) as representations of unitary groups. This approach follows the model proposed independently by Gell-Mann and Néeman and developed later in the works of Okubo, Gürsey and Radicati, Pais and other authors.

The book "Unitary symmetry theory" by Yu. Rumer and A. Fet was published in 1970, in which these ideas were discussed systematically. While working on the book, Rumer had an idea to apply the same approach to the system of chemical elements. After getting over some difficulties, we laid down a group systematization of elements in our joint work (Rumer and Fet, 1971). Already in this article, we emphasized that the approach implies considering symmetry as related to the atom as a whole rather than to its electron shells only. As a group symmetry, we chose a two-dimensional covering group of SO(4) group. In 1972, B. Konopel'chenko extended the symmetry group up to the conformal group (Rumer and Fet, 1971). Barut (1972) and Barrondo and Novaro (1972) independently described the symmetry from the viewpoint of electron shells.

Apparently, this clear differentiation between the symmetry of the elements and the traditional shell model helped us to achieve a clearer understanding of the obtained classification. In particular, I suggested a group description of chemical affinity in Fet (1974, 1975), and a mass formula for atoms in Fet (1979a, 1981). While refining the classification, we noticed, apparently for the first time, that the properties of elements change with some regularity. In particular, each p-, d-, and f-family is distinctly divided into two subfamilies where the properties of the elements change by different laws. The results were compared with experimental data by Byakov et al. (1976) and later, with additional material, by Sorokin.

Discussions of the method in scientific articles usually imply a sufficient knowledge of Lee groups. However, physicists and chemists usually meet in practice only representations of the three-dimensional rotation group, as it was elaborated by Wigner and Weil in the late 1920s. That is why I wanted to write a book that will be useful for this broad audience rather for a narrow circle of theorists. The work met serious difficulties since the available literature on Lee groups did not provide easy understanding of the ideas of symmetry which have acquired much importance in the Physics these last decades. What we have in this area are either systematic treatises for expert mathematicians or manuals for physicists which imitate these treatises or offer a number of separate applications to special cases. Therefore, I tried to state the main concepts of group theory and Lee algebras briefly, and only as far as it is

necessary to understand the symmetry of particles assuming that the reader has physical or chemical education and some basic knowledge of quantum mechanics. Group theory is explained from the very beginning, starting from the definition of a group. However, it would be desirable for the reader to have some preliminary idea of using rotation group for classification of atomic and molecular energy spectra. Group methods are introduced as necessary and are always illustrated by physical examples. Especially, the physical background of spin and unitary spin is discussed in detail. Therefore, the presentation of the material is "genetic" and inductive rather than deductive, that is, the main attention is paid to the origin and meaning of the concepts rather to the formal exactness of the constructions. In particular, mathematical rigor, though followed when possible, is not an end in itself. We cite only those theorems which are constantly used further, their meaning is discussed in detail but the proofs are usually omitted as well as cumbersome calculations which are cited, when necessary, in the Appendices.

First chapter of this book is an introduction to quantum chemical group methods and starts with the traditional applications of the rotation group to the hydrogen atom. Then a classical, though not broadly known, work of Vladimir Fock (1935) is discussed to demonstrate how hydrogen energy spectrum can be obtained from a four-dimensional rotation group. Since the work is very brief and not readily available nowadays, its most important part is considered in detail in Appendix A.

Second chapter shows how the observables of a quantum system can be obtained from its symmetry group. Thereby, symmetry groups are considered from the viewpoint of modern physics which implies that a quantum system is defined by the representation of a symmetry group. In particular, we discuss the relation between the Hamiltonian of the system and Casimir operators of its symmetry group.

Third chapter introduces the main ideas of Lee groups and algebras using physical background of the first two chapters. Each concept is illustrated with examples and is justified by detailed explanations.

Fourth chapter introduces the concepts of spin and isotopic spin, and explains the ideas of unitary symmetry. The discussion here, similar to the other chapters, implies the knowledge of simplest quantum mechanical concepts than some special literature. The concluding part of the chapter presents the main principles of classifying particles (or states) in a quantum theory and, I believe, contains some novelty when introducing a common principle of identifying similar particles in the multiplets of a symmetry group.

Chapters five and six present the main content of the book. They introduce the symmetry of the system of chemical elements illustrated by tables and graphs to compare the theory with experimental data.

I am very grateful to S. Prishchepionok who greatly contributed to improve the algebraic part of the book, and to N. Sorokin who did much work with the experimental material. In particular, Sorokin noticed that the suggested group classification provides good description of those properties which are associated with chemical

reactivity. Lately, this viewpoint was confirmed by Zhuvikin and Hefferlin (1983) who used our group method to explain regularities in the properties of diatomic molecules systematically studied by R. Hefferlin et al. (1979), Hefferlin and Kuhlman (1980), and Refferlin and Kutzner (1981). Unfortunately, I learned about these results after the book had been finished, and so the material was not included in this book.

January 9, 1984
Abram Fet

1 Symmetries of a quantum system

1.1 Rotation group in quantum mechanics

The motion of a particle is described in quantum mechanics by a function $\psi(x, y, z)$ of coordinates x, y, z and time t, which is called a *wave function of the particle*. Function ψ takes on complex values. In this chapter, we do not consider the spin of the particle and the change of its state with time; hence, ψ is a one-component function and its dependence on t is not indicated.

Mathematical apparatus of quantum mechanics does not allow a unique correspondence between a particle's state and some definite wave function: function ψ is defined for the given state with an accuracy up to a nonzero imaginary factor λ, so that ψ and $\lambda\psi$ represent the same state of the particle. The zero function ($\psi \equiv 0$) images no state. The wave function has a "probabilistic interpretation": the probability to find a particle in the domain D is proportional to the integral of $|\psi|^2$ over the domain D. Since for the whole space the probability is unity, all possible states of the particle are supposed to be defined by nonzero quadratically integrable functions:

$$\int |\psi(x, y, z)|^2 \, d^3x < \infty, \tag{1.1}$$

where $d^3x = dxdydz$, the integration is taken over the whole space, and every nonzero function satisfying eq. (1.1) defines the possible state of a particle. If we "normalize" ψ (by multiplying it with an appropriate factor) so that the integral (1.1) becomes equal to 1, the arbitrariness in the description is reduced to the phase factor $e^{i\varphi}$, where φ is real and does not depend on the coordinates. The phase factor does not change the meaning of ψ, since all numerical values derived from the quantum theory do not depend on it. For the normalized wave function ψ, the probability of finding the particle in D is

$$\int_D |\psi(x, y, z)|^2 \, d^3x \tag{1.2}$$

It can be shown that all quadratically integrable ψ functions constitute a linear space, that is, the sum and any complex multiple of such functions are also quadratically integrable. By analogy with the vectors of elementary geometry, objects that can be summed up and multiplied by a number are often referred to as *vectors*; therefore, ψ function is often called a *state vector* of the particle, and the linear space of all wave functions is called a *vector space*. Since linear combinations of wave functions are also wave functions (if they are not zero), the linear space of wave functions is equivalent to the so-called "principle of superposition", stating that a superposition of physically possible states is again a physically possible state of a quantum system.[1]

1 As we will see, this principle has some restrictions in more complex cases.

We assume in this chapter that the particle is not free and is placed in the electromagnetic field to act on its charge e. In this case, the *quantum system* is a particle in the field (e.g. classically defined as a central electrostatic field) rather than a particle per se. External factors (e.g. a photon absorption or emission, which is not described by the quantum mechanics of a *single* particle) can transform the system from state ψ into state φ. The probability of such transition is $|\langle\psi|\varphi\rangle|^2$, where

$$\langle\psi|\varphi\rangle = \int \psi^*(x,y,z)\varphi(x,y,z)d^3x \tag{1.3}$$

This expression is called the *scalar product* of the wave functions ψ and φ; we can show that the integral (1.3) is always finite. The scalar product (1.3) is *positive definite*, that is, $\langle\psi|\varphi\rangle > 0$ when $\psi \neq 0$. A vector space with a positive definite scalar product is called a *Hilbert space*; so the set of all wave functions constitutes a Hilbert space. The *norm* of function ψ is defined as the square root of the integral (1.1). The norm is used to define the convergence of series: a series $\psi_1 + \psi_2 + \ldots + \psi_n + \ldots$ is said to converge to ψ_0, if the norm $\psi_0 - s_n$ of its partial sum $s_n = \psi_1 + \ldots + \psi_n$ tends to zero.

Suppose now that the whole quantum system (a particle in the field) rotates about the coordinate origin. Let $\psi(x,y,z)$ describes the initial state of the system and $\psi'(x,y,z)$ describes its rotated state. Since the space is isotropic (all directions are equal), we assume that functions ψ and ψ' describe physically equivalent situations. Consider, for example, the region D in the proximity of point (x, y, z) with the volume d^3x. The probability to find the particle in the initial state of the system in this area is $|\psi(x,y,z)|^2 d^3x$. If the rotation O carries point (x, y, z) into (x', y', z'), and area D into D' with the volume d^3x', the probability to find the particle in the rotated state in D' is $|\psi'(x',y',z')|^2 d^3x'$. Sine the situations are equivalent, the following probabilities coincide:

$$|\psi(x,y,z)|^2 d^3x = |\psi'(x',y',z')|^2 d^3x' \tag{1.4}$$

Since $d^3x = d^3x'$, we have

$$|\psi'(x',y',z')| = |\psi(x,y,z)| \tag{1.5}$$

The simplest way to satisfy eq. (1.5) is to assume

$$\psi'(x',y',z') = \psi(x,y,z) \tag{1.6}$$

There is also another argument in favor of eq. (1.6). Transition probabilities $\psi \to \varphi$ (in the initial state) and $\psi' \to \varphi'$ (in the rotated state) should also be considered. Therefore, for any ψ, φ,

$$|\langle\psi|\varphi\rangle|^2 = \left|\int \psi^*(x,y,z)\varphi(x,y,z)d^3x\right|^2 = \left|\int \psi^{*\prime}(x',y',z')\varphi'(x',y',z'')d^3x\right|^2 = |\langle\psi'|\varphi'\rangle|^2 \tag{1.7}$$

From eq. (1.7), it can be mathematically deduced that $\psi'(x',y',z') = e^{i\varphi}\psi(x,y,z)$ where the phase factor may depend on ψ, but not on the coordinates. Again, the easiest way to satisfy this requirement is to assume eq. (1.6), that is, that all phase factors are equal to 1.

Equation (1.6) is a general law to describe the rotations of wave functions.

We have deduced the law (eq. 1.6) to describe *different* states of a quantum system (before and after the rotation) using the same system of coordinates (x, y, z) for the wave functions of the initial state $\psi(x, y, z)$ and the rotated state $\psi'(x, y, z)$. This is an *active* approach interpreting x', y', z' as the coordinates of another point in the same coordinate system.

There is another interpretation of eq. (1.6), which states that $\psi(x, y, z)$ and $\psi'(x', y', z')$ specify *the same* state of a quantum system in different coordinate systems. Since observations in these coordinate systems should identically describe experimental facts (e.g. the probability to find a particle in some region or the probability of some transition), the same quantum-mechanical procedure should derive the same values of observables from the wave functions. This leads to eqs. (1.4) and (1.7) and, consequently, to eq. (1.6). In many physical problems, this approach which is equivalent to the previous one is called "*passive*." However, in more complex situations, where state vectors describe "internal degrees of freedom" of the system rather than its space-time properties, we can no longer address the "reference system" or the "observer." Since we are interested exactly in such situations, we will usually use the *active* viewpoint; that is, assume that the method of mathematical description of the states is fixed, and the *states* of the system are transformed.

Rotation O is given by a linear homogeneous coordinate transform with orthogonal matrix $O = (o_{ij})$:

$$\begin{aligned} x' &= o_{11}x + o_{12}y + o_{13}z \\ y' &= o_{21}x + o_{22}y + o_{23}z \\ z' &= o_{31}x + o_{32}y + o_{33}z \end{aligned} \tag{1.8}$$

Designate point (x, y, z) as x and point (x', y', z') as x'. Then the rotation is written as $x' = Ox$, and eq. (1.6) as $\psi'(Ox) = \psi(x)$. To express ψ' directly through x, y, z, apply the reverse rotation O^{-1} and replace x in eq. (1.8) by $O^{-1}x$:

$$\psi'(x) = \psi(O^{-1}x) \tag{1.9}$$

or, expressing coordinates $O^{-1}x$ in terms of x using the orthogonal rotation matrix $O^{-1} = (o_{ij}^{-1})$, obtain the same as

$$\psi'(x, y, z) = \psi(o_{11}^{-1}x + o_{12}^{-1}y + o_{13}^{-1}z, o_{21}^{-1}x + o_{22}^{-1}y + o_{23}^{-1}z, o_{31}^{-1}x + o_{32}^{-1}y + o_{33}^{-1}z) \tag{1.10}$$

Therefore, each rotation O is related to some transform of wavefunctions (eq. 1.9) or, in other words, to some operator T_O which acts on ψ functions:

$$\psi' = T_O\psi \tag{1.11}$$

Operator T_O is said to *represent* rotation O in the space of wavefunctions R.

The most important property of representing operators is that they, like rotations, constitute a *group*. To remind the definition of the group, it is a set of elements G

satisfying the following conditions: there is a multiplication operation g_1g_2 defined on G and γ the association law $(g_1g_2)g_3 = g_1(g_2g_3)$, and there is an unit element e such that $ge = eg = g$ for any g from G, and for each g, there is an inverse element g^{-1} such that $gg^{-1} = g^{-1}g = e$.

Transformation or operator groups are often considered as acting in some space, and the multiplication of operators is defined as their sequential action: T_1T_2 designates the operator obtained as the result of the operator T_2 and then operator T_1, so

$$\mathrm{T}_3 = \mathrm{T}_1\mathrm{T}_2 \text{ means that if } T_2a = b,\ \ T_1b = c,\ \text{ then } T_3a = c \tag{1.12}$$

Associative law for multiplication of operators is satisfied automatically, since the action of T_3 followed by T_1T_2 means the same as the action of T_2T_3 followed by T_1 (in both cases, we need only to apply T_3, T_2, and T_1 in the specified order). The identity operator does not change the points of space. Designating the operator as 1, obtain $1(a) = a$. Evidently, $T \cdot 1 = 1 \cdot T = T$. The inverse operator T^{-1} acts inversely to T:

$$\text{if } Ta = b,\ \text{ then } T^{-1}b = a \tag{1.13}$$

Therefore, to verify if some operators constitute a group, we need to check if the product of such operators is the operator of the same kind, and that each of them has the inverse operator of the same kind.

Consider from this viewpoint rotations of the three-dimensional space O and the operators of rotation T_O. Evidently, successive rotations – that is, distance preserving transforms of the three-dimensional space – are again a transform of the same kind. Multiplication of rotations is associated with multiplication of matrixes (o_{ij}) to represent them in the given coordinate system. The unity rotation is imaged by the identity transformation with the identity matrix. Finally, each rotation O has the inverse rotation O^{-1} with the inverse matrix. Therefore, rotations of the three-dimensional space constitute a group (denoted by O(3)). We are interested in a smaller group or a *subgroup* of $O(3)$ consisting of proper rotations, that is, those which do not change the orientation of the space (the determinant of their matrices is +1). The group of proper rotations of the three-dimensional space is denoted as $SO(3)$.[2] Henceforth, when talking about rotations, we mean proper rotations only.

Let O_1, O_2 be rotations and $O_3 = O_1O_2$. Accomplish successively operators T_{O_2} and T_{O_1} (eq. (1.9)):

$$T_{O_2}\psi = \psi',\ \text{ where } \psi'(x) = \psi(O_2^{-1}x),\ \ T_{O_1}\psi' = \psi'',\ \text{ where } \psi''(x) = \psi'(O_1^{-1}x) \tag{1.14}$$

Substituting $O_1^{-1}x$ instead of x in the definition of ψ', obtain

$$\psi'(O_1^{-1}x) = \psi(O_2^{-1}(O_1^{-1}x)) = \psi(O_2^{-1}O_1^{-1}x) = \psi((O_1O_2)^{-1}x),$$

2 Spécial orthogonal.

and from the definition of ψ''

$$\psi''(x) = \psi(O_3^{-1}x) \tag{1.15}$$

Equation (1.15) means that successive application of operators T_{O_2} and T_{O_1} to the function ψ'' is equivalent to a single application of operator T_{O_3}; in other words,

$$T_{O_1 O_2} = T_{O_1} T_{O_2} \tag{1.16}$$

Thus, representing operators of rotations are multiplied *in the same order* as the rotations. At the same time, it was found that the product of operators is again a rotation operator. Substituting this in eq. (1.16), O_1^{-1} instead of O_2, obtain $T_O T_{O^{-1}} = 1$. Therefore, $T_{O^{-1}}$ is inverse to T_O:

$$T_{O^{-1}} = (T_O)^{-1} \tag{1.17}$$

Thus, the inverse operator of rotation is again the operator of rotation, and all such operators T_O constitute a group. If, in general, the elements of some group g are associated with operators T_g acting in some space, so that

$$T_{g_1 g_2} = T_{g_1} T_{g_2}, \quad T_e = 1, \tag{1.18}$$

then we say that a *representation* of group G is defined in this space. Representation is a method to image a group by the group of operators. When different elements g correspond to different operators T_g, the representation is *faithful*. In this case, the group of operators is *isomorphic* to the initial group, that is, the replacement of g by T_g changes only the *type* of elements rather than the algebraic multiplication law. It can be shown that the representation of the rotation group $\{T_O\}$ is faithful.

As we will show, operators T_O are *linear*. In general, linear operators T are those which carry a sum into a sum and a multiple into a multiple:

$$T(\psi_1 + \psi_2) = T\psi_1 + T\psi_2, \quad T(\lambda\psi) = \lambda T\psi \tag{1.19}$$

According to eq. (1.9), $\psi_1' = T\psi_1$ is defined as $\psi_1'(x) = \psi_1(O^{-1}x)$, and, similarly, $\psi_2'(x) = \psi_2(O^{-1}x)$; therefore, $\psi_1'(x) + \psi_2'(x) = \psi_1(O^{-1}x) + \psi_2(O^{-1}x)$; the same is obtained if $O^{-1}x$ is substituted in the sum $\psi_1(x) + \psi_2(x)$ instead of x. So, $T_O\psi_1 + T_O\psi_2 = T_O(\psi_1 + \psi_2)$. The same is true for eq. (1.19).

Representation $\{T_g\}$ of a group G is *linear* if operators T_g are linear and are defined on a vector space. Furthermore, when talking about representations, we always mean linear representations without mentioning their linearity.

Furthermore, operators T_O are *unitary*. A linear operator T in a Hilbert space is unitary if it preserves scalar products:

$$\langle T\psi | T\varphi \rangle = \langle \psi | \varphi \rangle \quad \text{for all } \psi, \ \varphi \tag{1.20}$$

In our case, taking $\psi' = T_O\psi$ and $\varphi' = T_O\varphi$, we obtain

$$\langle \psi' | \varphi' \rangle = \int \psi'^*(x)\varphi'(x)d^3x = \int \psi^*(O^{-1}x)\varphi(O^{-1}x)d^3x.$$

After changing the variables $O^{-1}x = x'$ and since the Jacobian $\left|\frac{dx'}{dx}\right| = 1$, we obtain

$$\int \psi^*(x')\varphi(x')d^3x' = \langle\psi|\varphi\rangle,$$

which was to be proved.

Representation $\{T_g\}$ of a group G is *unitary*, if operators T_g are unitary and are defined in a Hilbert space. As we can see, our representation $\{T_O\}$ is unitary. We will discuss in detail the role of unitary representations in Physics.

The first application of group theory in quantum mechanics was associated with the calculation and studying of eigenfunctions of the energy operator H. In the case of a general spherically symmetric potential of a charged particle, the Hamiltonian has the form

$$H = \frac{1}{2m}p^2 + V(r). \tag{1.21}$$

This operator commutes with all operators of rotation T_O,

$$T_O H = HT_O, \tag{1.22}$$

that is, both products are identical; in other words, for any function ψ, action H followed by T_O gives the same function as action T_O followed by H. Obviously, it will be sufficient to prove it for operators p^2 and V. Let $T_O\psi = \psi'$. Then from eq. (1.10), we have

$$p_x\psi' = \frac{\hbar}{i}\frac{\partial}{\partial x}\psi' = \frac{\hbar}{i}\left(o_{11}^{-1}\frac{\partial\psi}{\partial x} + o_{21}^{-1}\frac{\partial\psi}{\partial y} + o_{31}^{-1}\frac{\partial\psi}{\partial z}\right), \tag{1.23}$$

and similarly for p_y and p_z. As $p^2 = p_x^2 + p_y^2 + p_z^2$, matrix O^{-1} is orthogonal; reapply the momentum operators and easily obtain $p^2\psi' = (p^2\psi)'$, where the prime on the right side means the substitution of arguments (1.10). Further, $V(r)\psi'(x)$ is obtained by multiplying $V(r)$ by $\psi(O^{-1}x)$; but, as the distance r does not change during the rotation, we obtain the same if $O^{-1}x$ is substituted in $V(r)\psi(x)$ instead of x.

Let ψ be an eigenfunction of the energy operator, that is, $H\psi = E\psi$. In this case, all functions $\psi' = T_O\psi$ obtained from ψ by rotations are also eigenfunctions of H with the same eigenvalues E. This is to be expected from symmetry reasons since states ψ and ψ' differ only in the spatial orientation of the quantum system, which cannot change the energy of the system in a spherically symmetric field. The formal verification is as follows:

$$H\psi' = HT_O\psi = T_O H\psi = T_O(E\psi) = ET_O\psi = E\psi' \tag{1.24}$$

Therefore, a group of transforms commuting with the energy operator makes it possible to obtain eigenfunctions $\psi_1 = T_{O_1}\psi_0, \psi_2 = T_{O_2}\psi_0, \ldots$ from a single eigenfunction ψ_0; it can be proved that only a finite number of them are linearly independent. By choosing appropriate O_1, O_2, we can obtain eigenfunctions as the following linear combinations:

$$c_1\psi_1 + \ldots + c_k\psi_k \tag{1.25}$$

Therefore, the eigenvalue E is k-fold degenerate, which can be revealed by "removing the degeneracy," for example, by applying a magnetic field. A representation of the rotation group $\{T_O\}$ makes it possible to find from a single eigenfunction the basis of eigenfunctions $\psi_1, \ldots, \psi_k$ with the same eigenvalue and to evaluate the multiplicity of the eigenvalue, which turns out to be *not less* than k.

Consider the concept of the *invariant subspace* of a representation. Let $\{T_g\}$ be a representation of group G. If a subspace W of the representation space is such that for any vector φ from W, all vectors $T_g\varphi$ also belong to W, then W is called an invariant subspace of representation $\{T_g\}$. In other words, the subspace is invariant if the representation operators act only inside it and thus define a "restricted" representation of group G on the space W. As is seen from eq. (1.24), *all* eigenfunctions of energy operator (eq. 1.21) having the same eigenvalue E constitute an invariant subspace of representation $\{T_O\}$ of the rotation group. It can be shown that such subspaces W_E are finite, that is, all their vectors are expressed in terms of a finite basis.

Linear combinations (eq. 1.25) obtained from a *single* eigenfunction by rotation operators also constitute an invariant subspace:

$$\begin{aligned} T_O(c_1\psi_1 + \cdots + c_k\psi_k) &= T_O(c_1T_{O_1}\psi_0 + \cdots + c_kT_{O_k}\psi_0) = c_1T_OT_{O_1}\psi_0 + \cdots + c_kT_OT_{O_k}\psi_0 \\ &= c_1T_{O\,O_1}\psi_0 + \cdots + c_kT_{O\,O_k}\psi_0 \end{aligned} \tag{1.26}$$

But $T_{O\,O_j}\psi_0$ are expressed in terms of $\psi_1, \ldots \psi_\kappa$, which are the basis for all functions $T_O\psi_0$, so the right-hand side can be represented in the same form (eq. (1.25)). We denote this subspace W_{ψ_0}. Evidently, W_{ψ_0} is a subset of W_E.

In the general case, potential $V(r)$ is of arbitrary form and the eigenspace W_E contains no smaller invariant subspace of representation $\{T_O\}$; such invariant space is called *irreducible*. (Appendix B describes the structure of all irreducible subspaces of the rotation group.) If W_E is irreducible, then W_{ψ_0} is also irreducible and $\mathsf{W}_E = \mathsf{W}_{\psi_0}$. Therefore, in the general case, eigenspaces of a spherically symmetric energy operator can be obtained simply by applying rotation operators T_O to some eigenfunction and then by constructing linear combinations of these new eigenfunctions. From the dimension of space W_{ψ_0}, we can estimate the "inevitable" degeneracy of the energy eigenvalue E. In such important cases as, for example, the Coulomb potential, the space can be reducible, and its dimension exceeds the above estimation. Such degeneration is called "accidental degeneration." For now, we leave aside "accidental degenerations" and consider only irreducible eigensubspaces of energy W_E. We also assume that far from the germ, the Hamiltonian little differs from the Coulomb Hamiltonian, that is,

$$H = H_0 + H_1, \text{ where } H_0 = \frac{1}{2m}p^2 - \frac{Ze^2}{r} \text{ and } H_1 = V(r), \tag{1.27}$$

where matrix elements of $V(r)$ are small as compared to H_0, and $V(r)$ decreases quite rapidly at infinity. These conditions are true for the approximate model of a multi-electron atom implying that the energy of a single electron is calculated, and all other electrons are replaced by a spherically symmetric charged layer which "screens" the nucleus.

We are interested only in the wave functions of *bounded* electron states, that is, the states where the electron is not removed to infinity. All such functions are expanded in terms of the eigenfunctions of the energy operator with negative eigenvalues. Furthermore, we will consider only such wavefunctions and denote their space R. Scattering problems of unbounded electrons are not considered in this book, and "wavefunctions" are assumed to describe bounded states only.

In the above conditions, we can build in space R a complete orthonormal basis of eigenfunctions of operator H, as it is done in the textbooks on quantum mechanics,

$$\psi_{nlm}(x, y, z) = f_n(r)Y_l^m(\upsilon, \varphi), \tag{1.28}$$

where the "principal quantum number" n takes values 1, 2,…; "azimuthal quantum number" l for a given n takes values 0, 1,…, $n-1$; and "magnetic quantum number" m for a given l takes values $-l, -l+1, \dots, l-1, l$. "Radial functions" $f_n(r)$ decrease exponentially when $r \to \infty$, and $Y_l^m(\upsilon, \varphi)$ are spherical functions defined on the sphere $S^2(x^2 + y^2 + z^2 = 1)$.

Eigenfunctions (eq. 1.28) are connected to eigenvalues E_{nl} which depend on integer parameters n, l (but not on m). If there is no "accidental degeneracy," all values E_{nl} are different. Any wave function ψ is uniquely expanded into a series of eigenfunctions of H:

$$\psi = \sum_{n,l,m} c_{nlm}\psi_{nlm} \tag{1.29}$$

Combine the terms with the same values n and l and denote the obtained sums ψ_{nl}; then the wavefunction is expanded into the series

$$\psi = \sum_{n,l} \psi_{nl} \tag{1.30}$$

with orthogonal terms, where ψ_{nl} are eigenfunctions of H connected to eigenvalues E_{nl}, that is, they belong to the eigensubpace $\mathsf{W}_{E_{nl}}$. Therefore, eq. (1.30) defines the expansion of the space of all wave functions R into the *orthogonal sum* of irreducible invariant subspaces of $\mathsf{SO}(3)$ group (denoted, for brevity, R_{nl}):

$$\mathsf{R} = \oplus \mathsf{R}_{nl}. \tag{1.31}$$

Basis R_{nl} consists of functions (eq. 1.28) with fixed n, l, and variable m. Rotation T_O does not change factor $f_n(r)$ and, as can be shown, carries spherical function $Y_l^{(m)}$ into a linear combination of spherical functions with the same n, l, and $m = -l, -l+1, \dots, l-1, l$.

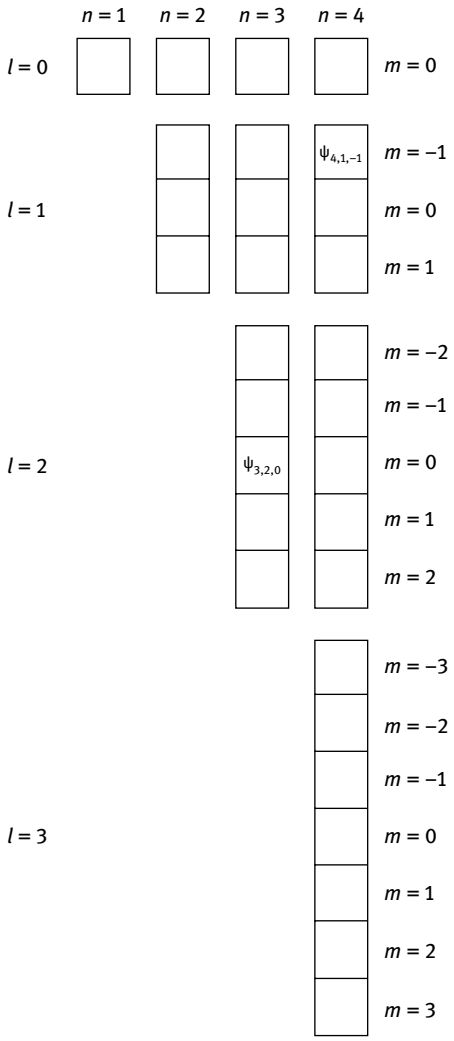
If H is a Coulomb potential ($H = H_0$), eigenvalues E_{nl} do not depend on l (and are denoted as E_n). Combining in eq. (1.29) all terms with the same n and denoting W_{E_n} as R_n, obtain the orthogonal decomposition

$$\psi = \sum_{n=1}^{\infty} \psi_n \tag{1.32}$$

and

$$\mathsf{R} = \mathsf{R}_1 \oplus \mathsf{R}_2 \oplus \cdots \oplus \mathsf{R}_n \oplus \cdots \tag{1.33}$$

Table 1.1: Expansion of R into irreducible subspaces.



Invariant subspace R_{nl} has a basis consisting of eigenfunctions (eq. 1.28) with $m = -l, -l+1, \ldots, l-1, l$; hence, its dimension is $2l+1$. Invariant subspace

$$\mathsf{R}_n = \mathsf{R}_{no} \oplus \cdots \oplus \mathsf{R}_{n,n-1} \tag{1.34}$$

has a basis constituted by bases of all ψ_{nlm} with given n; its dimension is

$$\sum_{l=0}^{n-1} (2l+1) = n^2 \tag{1.35}$$

Expansion (1.34) is possible also in the case of a general potential $V(r)$, but functions R_n will not be eigenfunctions of H; rather, they will be linear combinations of eigenfunctions having the same radial function $f_n(r)$. Since all terms in eq. (1.34) are invariant subspaces, the sum of their R_n is also an invariant subspace though not an eigensubpace of H.

Expansion of R into irreducible subspaces is conveniently represented by the following table, where the cells correspond to the basis functions ψ_{nlm} (Fig. 1.1). Rectangles of Table 1.1 depict *irreducible* subspaces R_{nl} of SO(3) group. Basis vectors corresponding to cells of the same rectangle are "connected" by representation operators $\{T_O\}$ in the sense that each of them can be obtained from any other by operators T_{O_i} and linear combinations (see eq. (1.25)). Vertical columns represent invariant spaces R_n. Rotation operators T_O connect neither different rectangles nor different columns, but "work" inside the rectangles. To connect *all* cells of Table 1.1, we need to *extend* SO(3) group, which will be done later. The representation of the extended group will have enough operators to achieve this goal and will be irreducible on the whole space of wavefunctions R.

1.2 Electron in the Coulomb field

Now consider in detail the electron in a Coulomb field. If the charge of the nucleus is $Z|e|$, eigenfunctions and eigenvalues of the energy operator H_0 are defined by the equation

$$-\frac{\hbar^2}{2m}\Delta\psi - \frac{Ze^2}{r}\psi = E\psi. \tag{1.36}$$

Eigenvalues H_0 depend only on the principal quantum number n and are written as

$$E_n = -\frac{Z^2me^4}{2\hbar^2}\frac{1}{n^2} \tag{1.37}$$

As mentioned in Section 1.1, eigenfunctions ψ_{nlm} belong to E_n and form a n^2-dimensional space R_n which decomposes into the orthogonal sum of subspaces R_{nl} ($l = 0, 1, \ldots, n-1$) with dimensions $1, 3, 5, \ldots, 2n-1$ (see eq. (1.33)). Each space R_{nl} is irreducible for the rotation group, but R_n are reducible (for $n > 1$). Therefore,

the order of eigenvalue E_n cannot be explained by the spherical symmetry of the Hamiltonian in contrast to the case of the general potential $V(r)$ when the eigenvalues $E_{nl}(l = 0, 1, \dots, n-1)$ do not coincide and their multiplicities are the dimensions of the corresponding representations of SO(3). This, so-called "accidental degeneracy" was explained in 1935 for the Coulomb potential by V.A. Fock with the help of a group theoretical approach (Fock, 1935, 1936). Fock's work, born far before its time, is not enough known and is currently hardly accessible. A part of it, which we will need, is discussed in detail in Appendix A, and here we present its final results only.

As is known, the state of an electron can also be described in the momentum representation by function $\widetilde{\psi}(p_x, p_y, p_z)$ related to $\psi(x, y, z)$ by Fourier transform:

$$\begin{aligned}\widetilde{\psi}(p_x, p_y, p_z) &= (2\pi\hbar)^{-3/2}\int \psi(x, y, z)e^{-i(p_x x+p_y y+p_z z)/\hbar}d^3x,\\ \psi(x, y, z) &= (2\pi\hbar)^{-3/2}\int \widetilde{\psi}(p_x, p_y, p_z)e^{i(p_x x+p_y y+p_z z)/\hbar}d^3p.\end{aligned} \tag{1.38}$$

Denote the Fourier operators in eq. (1.38) U and U^{-1}:

$$\widetilde{\psi} = U\psi, \quad \psi = U^{-1}\widetilde{\psi}. \tag{1.39}$$

Operators U and U^{-1} are linear and preserve scalar products $\langle\psi|\varphi\rangle$:

$$\langle\widetilde{\psi}|\widetilde{\varphi}\rangle = \langle\psi|\varphi\rangle. \tag{1.40}$$

A linear one-to-one correspondence between vectors of Hilbert spaces preserving scalar products is called an *isomorphism*. Thus, space R of functions $\psi(x, y, z)$ and space $\widetilde{\mathsf{R}}$ of functions $\widetilde{\psi}(p_x, p_y, p_z)$ (with scalar product similar to eq. (1.3)) are isomorphic. Under the isomorphism, eigenfunctions of H_0 from eq .(1.36) transform into the solutions of the integral,

$$\frac{1}{2m}p^2\widetilde{\psi}(p) - \frac{Ze^2}{2\pi^2\hbar}\int\frac{\widetilde{\psi}(p')d^3p'}{|p'-p|^2} = E\widetilde{\psi}(p), \tag{1.41}$$

where $d^3p' = dp'_x dp'_y dp'_z$ and the integration extends over the whole momentum space (all proofs see in Appendix A). As U preserves the orthogonality and the dimension, subspaces $\widetilde{\mathsf{R}}_n = U\mathsf{R}_n$ composed of eigenfunctions of eq. (1.41) associated with eigenvalues E_n are orthogonal to each other and have the same dimension n^2.

Since basis $\psi_{nlm}(x)$ transforms into basis $\widetilde{\psi}_{nlm}(p)$ of space $\widetilde{\mathsf{R}}$, the structure of eigenfunctions in $\widetilde{\mathsf{R}}$ is the same as in R.

Fock translates the momentum space (p_x, p_y, p_z) into the sphere S^3

$$\xi_1^2 + \xi_2^2 + \xi_3^2 + \xi_4^2 = 1 \tag{1.42}$$

of a four-dimensional *Euclidean* space R^4 with distances between its points:

$$|\xi - \eta| = [(\xi_1 - \eta_1)^2 + (\xi_2 - \eta_2)^2 + (\xi_3 - \eta_3)^2 + (\xi_4 - \eta_4)^2]^{1/2} \tag{1.43}$$

(this space should not be confused with the Minkowski space having a nonpositive metric form used in the special theory of relativity). Coordinates ξ_k have no relation to space–time coordinates and no physical meaning. The points on S^3 are described by three independent parameters only, because the four coordinates on the sphere are connected by eq. (1.42); therefore, the sphere S^3, similar to the momentum space, is *three-dimensional* (the superscript denotes the dimension).

Since eigenvalues E are negative for bound states (eq. (1.45)), the number

$$p_0 = \sqrt{-2mE} \tag{1.44}$$

is positive (and equals the mean square of the momentum p^2 in the state $\widetilde{\psi}(p)$). Correspondence between the points $p = (p_x, p_y, p_z)$ of momentum space and points $\xi = (\xi_1, \xi_2, \xi_3, \xi_4)$ of the sphere S^3 is defined as follows:

$$\begin{aligned}
\xi_1 &= \frac{2p_0 p_x}{p^2 + p_0^2} = \sin\alpha \sin\vartheta \cos\varphi \\
\xi_2 &= \frac{2p_0 p_y}{p^2 + p_0^2} = \sin\alpha \sin\vartheta \sin\varphi \\
\xi_3 &= \frac{2p_0 p_z}{p^2 + p_0^2} = \sin\alpha \cos\vartheta \\
\xi_4 &= \frac{p^2 - p_0^2}{p^2 + p_0^2} = \cos\alpha
\end{aligned} \tag{1.45}$$

where α, ϑ, and φ are the spherical coordinates on S^3 similar to usual coordinates ϑ and φ on $S^2 (0 \le \alpha \le \pi, 0 \le \vartheta \le \pi, 0 \le \varphi \le 2\pi)$. The geometric meaning of eq. (1.45) as a four-dimensional "stereographic projection" is explained in Appendix A. It is easily verified that eq. (1.42) is true for any p_x, p_y, p_z, so we actually obtain the points of S^3.

Furthermore, following Fock's reasoning, the correspondence between the eigenfunctions $\widetilde{\psi}(p)$ of eq. (1.41) and the functions on the three-dimensional sphere is defined as follows:

$$\Psi(\alpha, \vartheta, \varphi) = \frac{\pi}{\sqrt{8}} p_0^{-5/2} (p^2 + p_0^2)^2 \widetilde{\psi}(p), \tag{1.46}$$

where $\alpha, \vartheta, \varphi$ are defined from eq. (1.45) by the set (p_x, p_y, p_z), and p_0 is given by eq. (1.44). Equation (1.41) for $\widetilde{\psi}(p)$ can be rewritten as the integral for Ψ:

$$\Psi(\alpha, \vartheta, \varphi) = \frac{\lambda}{2\pi^2} \int \frac{\Psi(\alpha', \vartheta', \varphi') d\Omega'}{|\xi' - \xi|^2}, \tag{1.47}$$

where $d\Omega' = \sin^2\alpha' \sin\vartheta' d\alpha' d\vartheta' d\varphi'$ is an element of S^3, the integration is taken over the whole sphere, $2\pi^2$ is the area of S^3, and distance $|\xi - \xi'|$ is expressed in terms of $\alpha, \vartheta, \varphi, \alpha', \vartheta', \varphi'$ with the help of eqs. (1.43) and (1.45); finally, we have

$$\lambda = \frac{Zme^2}{\hbar\sqrt{-2mE}} \tag{1.48}$$

Let $E = E_n$. Then ψ belongs to the subspace R_n, and from eqs. (1.37) and (1.48), we find $\lambda = n$. Thus (including the factor $1/2\pi^2$ in the integral operator), we can see that $\Psi(\xi)$ is an eigenfunction of the integral eq. (1.47) with eigenvalue n.

A scalar product on the sphere S^3 is defined as

$$\langle\Psi|\Phi\rangle = \frac{1}{2\pi^2}\int \Psi^*(\alpha, \vartheta, \varphi)\Phi(\alpha, \vartheta, \varphi)d\Omega\,. \tag{1.49}$$

It can be verified that the Fock's transform $\widetilde{\psi}(p) \to \Psi(\xi)$ preserves the scalar products:

$$\langle\Psi|\Phi\rangle = \langle\widetilde{\psi}|\widetilde{\varphi}\rangle \tag{1.50}$$

Comparing this with eq. (1.40), we see that a consecutive transform $\psi(x) \to \widetilde{\psi}(p) \to \Psi(\xi)$ defines operator F_n as

$$\Psi = F_n\psi, \tag{1.51}$$

which is linear, preserves scalar products, and transforms the space of eigenfunctions R_n belonging to the eigenvalues E_n of Schrödinger equation (eq. (1.36)) into a set of eigenfunctions of Fock's integral (eq. (1.47)) belonging to the eigenvalue n. This way, we can obtain *all* eigenfunctions of eq. (1.47) with the eigenvalue n. Denoting the space of such functions F_n, eq. (1.51) is an isomorphism between R_n and F_n.

Space F_n is very simple to describe. It consists of *four-dimensional spherical functions* of order $(n - 1)$. To define them, a well-known method of constructing usual (three-dimensional) spherical functions is used. Consider the homogeneous polynomials of x, y, z of order l, satisfying the Laplace equation:

$$\Delta u_l(x, y, z) = 0 \tag{1.52}$$

For example, for $l = 0$, such polynomials are constants; for $l = 1$, the polynomials are $u_1 = x, y, z$; for $l = 2$, the polynomials are $u_2 = x^2 - y^2$ or $u_2 = yz$, and so on. On the sphere S^2, polynomials u_l are transformed into the so-called "spherical functions of order l"[3] $Y_l(\vartheta, \varphi)$. Functions $Y_l^m(\vartheta, \varphi)$, *where* $(m = -l, -l + 1, \ldots, l - 1, l)$, constitute a basis of the space of all spherical functions of order l, and the basis is orthogonal with respect to the integration over S^2. Since the Laplacian commutes with rotations (eq. (1.22)), operators T_o translate homogeneous harmonic polynomials of order l into polynomials of the same kind and, therefore, spherical functions of order l are carried into the functions of the same kind. This defines a representation of SO(3) in the space

3 The term "spherical function" does not imply all functions defined on the sphere; rather, these are only some functions of a special form. Their relation to the Laplace equation is marked by the term "spherical harmonics."

of spherical functions $Y_l(\vartheta, \varphi)$. Each of the basic spherical functions $Y_l^m(\vartheta, \varphi)$ is carried by operators T_o into a linear combination of the same basic functions (which are the basis of the representation space or, shorter, a *basis of the representation*). For wave-functions $\psi_{nl}(x, y, z) = f_n(r)Y_l(\vartheta, \varphi)$, transforms T_o essentially operate on Y_l, and $f_n(r)$ remains unchanged. Therefore, in the eigensubspace of the energy operator R_{nl}, generated by functions ψ_{nl} (eqs. (1.30) and (1.31)), the rotation group acts in the same way as in the space of spherical functions Y_l. This shows that the representation SO(3) in R_{nl} is independent of n.

Four-dimensional spherical functions are constructed in a similar way. Consider n-th order homogeneous polynomials of $\xi_1, \xi_2, \xi_3, \xi_4$, satisfying the four-dimensional Laplace equation:

$$\Delta^{(4)}u_n = \frac{\partial^2 u_n}{\partial \xi_1^{\,2}} + \frac{\partial^2 u_n}{\partial \xi_2^{\,2}} + \frac{\partial^2 u_n}{\partial \xi_3^{\,2}} + \frac{\partial^2 u_n}{\partial \xi_4^{\,2}} = 0 \tag{1.53}$$

These polynomials turn into four-dimensional spherical functions $Y_n(\alpha, \vartheta, \varphi)$ of order n on the sphere S^3. Spherical functions of order $(n-1)$ $(n = 1, 2, \ldots)$[4] can be shown to have a basis which is orthogonal with respect to integration over S^3 and consisting of functions

$$\Psi_{nlm}(\alpha, \vartheta, \varphi) = \Pi_{nl}(\alpha)Y_l^m(\vartheta, \varphi) \tag{1.54}$$

where $Y_l^m(\vartheta, \varphi)$ are ordinary spherical functions ($m = -l, -l+1, \ldots, l-1, l$), and l takes values $0, 1, \ldots, n-1$. The Fock transform carries the eigenfunctions $\psi_{nlm}(x, y, z)$ of the Schrödinger equation into four-dimensional spherical functions $\Psi_{nlm}(\alpha, \vartheta, \varphi)$ with the same indices.

Fock showed that the eigenfunctions of eq. (1.47) belonging to the eigenvalue $\lambda = n$ exactly coincide with four-dimensional spherical functions of $(n-1)$-th order $Y_{n-1}(\alpha, \vartheta, \varphi)$. In particular, the basis for these functions consists of the above functions Ψ_{nlm}. It is remarkable that Coulomb potential $1/r$ does not take part in this description of eigenfunctions. As we will see, a special form of the potential turns here into additional symmetry of the problem.

Fock transform F_n is constructed separately for each subspace R_n since eqs. (1.45) and (1.46) contain p_0 depending on E_n (eq. (1.44)). As we will see, we can construct from F_n $(n = 1, 2, \ldots)$ a single transform F of the space of all wave functions R into the space of all square-integrable functions on the sphere S^3; this Hilbert space is denoted as F and is called the *Fock space*.[5] Define F as taking the same values as F_n on the

4 We consider here spherical functions of order $(n-1)$ rather than order n, because they correspond to the eigenvalue n.

5 The other "Fock space" used in the quantum field theory is not considered in this book.

subspaces R_n, so that $F\psi_{nlm} = \Psi_{nlm}$; for wave functions which are not eigenfunctions of H_0, use eq. (1.32) and define

$$F\psi = \sum_{n=1}^{\infty} F_n\psi_n \tag{1.55}$$

Obviously, F is a linear operator. Since ψ_n and $F_n\psi_n$ are orthogonal to each other, we have

$$\langle F\psi|F\varphi\rangle = \left\langle \sum_n F_n\psi_n \middle| \sum_{n'} F_{n'}\psi_{n'} \right\rangle = \sum_n \langle F_n\psi_n|F_n\varphi_n\rangle \tag{1.56}$$

and since F_n preserves the scalar product, so does operator F. Furthermore, each square-integrable function $\Psi(\alpha, \vartheta, \varphi)$ can be expanded into four-dimensional spherical functions

$$\Psi = \sum_{n=1}^{\infty} \Psi_{n-1} \tag{1.57}$$

and, therefore, can be obtained by F from function

$$\psi = \sum_{n=1}^{\infty} F_n^{-1}(\Psi_{n-1}) \tag{1.58}$$

Thus, *operator F defines an isomorphism of the Hilbert space* R *of Schrödinger wave functions on the Hilbert space* F *of Fock wave functions*.

Isomorphic spaces can easily be used instead of each other in all aspects of quantum mechanics; the choice between them depends on the particular problem where they are most convenient to use. For example, the isomorphism of the Fourier transform allows performing various tasks in either coordinate or momentum representations, while the "Fock representation" is particularly useful to consider particles in the Coulomb field. As we will see, the group of four-dimensional rotations SO(4), greater than the rotation group of three-dimensional space SO(3), naturally acts on the space F.

1.3 Broken symmetry

Consider a rotation group in the four-dimensional Euclidean space R^4 with coordinates ξ_1, ξ_2, ξ_3, ξ_4. This is a group of homogeneous linear transforms preserving distances and written similar to eq. (1.8):

$$\begin{aligned} \xi'_1 &= o_{11}\xi_1 + \cdots + o_{14}\xi_4 \\ &\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots \\ \xi'_4 &= o_{41}\xi_1 + \cdots + o_{44}\xi_4 \end{aligned} \tag{1.59}$$

or, shorter, $\xi' = O\xi$. Here $O = (o_{ij})$ is an orthogonal matrix of the fourth order. Rotations, which do not change the orientation of the space, similar to that in the three-dimensional case, are given by the equation $\det|o_{ij}| = +1$.[6]

All such rotations constitute group SO(4). By analogy with eq. (1.9), define transforms of functions $\Psi(\xi) = \Psi(\xi_1, \xi_2, \xi_3, \xi_4)$ as

$$\Psi'(\xi) = \Psi(O^{-1}\xi) \tag{1.60}$$

or

$$\Psi'(\xi_1, \xi_2, \xi_3, \xi_4) = \Psi(o_{11}^{-1}\xi_1 + \cdots + o_{14}^{-1}\xi_4, \ldots, o_{41}^{-1}\xi_1 + \cdots + o_{44}^{-1}\xi_4) \tag{1.61}$$

Just as three-dimensional rotations, operators

$$\Psi' = T_O\Psi \tag{1.62}$$

are proved to define a *representation* of group SO(4) in the Fock space of functions $\Psi(\xi)$ (see eqs. (1.10), (1.14), and further). The difference is that functions $\Psi(\xi)$ are considered only on the sphere S^3 and are not defined in the whole space R^4, whereas Schrödinger wave functions $\psi(x, y, z)$ are defined in the whole three-dimensional space.

Operators T_O are easily verified to preserve the scalar product in F (eq. (1.49)); indeed, we can make a change of variables $O' = O^{-1}\xi$ in the integral

$$\langle\Psi'|\Phi'\rangle = \int \Psi'^*(\xi)\Phi'(\xi)d\Omega = \int \Psi^*(O^{-1}\xi)\Phi(O^{-1}\xi)d\Omega\,. \tag{1.63}$$

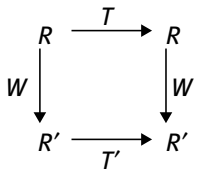
Since the area elements do not change on S^3 during rotations, $d\Omega' = d\Omega$, and the integral (1.63) equals $\langle\Psi|\Phi\rangle$. So, we have a *unitary* representation $\{T_O\}$ of group SO(4) in space F.

This representation is evidently *reducible* because orthogonal transforms of variables carry homogeneous harmonic polynomials $u_n(\xi_1, \xi_2, \xi_3, \xi_4)$ into polynomials of the same kind (similar to the polynomials of three variables), and thereby the subspaces of four-dimensional spherical functions F_n ($n = 1, 2, \ldots$) are invariant with respect to SO(4). However, these subspaces are *irreducible* for SO(4) (see Appendix B). Thus, SO(4) group connects, in the above sense, all basis vectors of each subspace F_n, or the cells of each vertical column of Table 1.1. But different columns of the table remain disconnected: SO(4) group "works" within the columns.

As mentioned above, space R of Schrödinger wave functions $\psi(x, y, z)$ and space F of Fock functions $\Psi(\xi_1, \xi_2, \xi_3, \xi_4)$ are isomorphic; however, the action of SO(4) group is obvious on the second of them, but not on the first, since $\psi(x, y, z)$ depends only on three variables. We will not describe here the representation of SO(4) on R, but

6 They translate any basis $(e_1, e_2, e_3, e_4)$of space R^4 into the basis (e'_1, e'_2, e'_3, e'_4) obtained from the initial basis by continuous deformation $e_k \to e_{k'}$, so that the vectors remain linearly independent (which means that the bases have the same orientation).

use the general concept of equivalent representations. Let R and R' be isomorphic spaces, W being the isomorphism between them. Then every operator T on R defines the operator T' on R', and vice versa; if $Ta = b$ in R, and $a' = Wa$ and $b' = Wb$ are the corresponding vectors in R', then $T'a' = b'$. In other words, operator T' reproduces the action of T on the "isomorphic images" of the vectors from R. This can be imaged as the following diagram:



(1.64)

The diagram says that if we take a vector a in R, apply to it the operator T and then take the image of the resulting vector $b = Ta$ for the isomorphism $a' = Wa$ (moving to the right and downward), the result will be the same as for the sequence of taking the image for the isomorphism $a' = Wa$, and then for $b' = T'a'$ (moving downwards and to the right). To construct T' from T, we need to find $a = W^{-1}a'$ for a given vector a' from space R' (moving upwards), then $b = Ta$ (moving to the right), and, finally, $b' = Wb$ (moving downwards). In short, it is written as

$$T' = WTW^{-1} \tag{1.65}$$

If a representation $\{T_g\}$ of group G is defined on R, we can construct corresponding operators on the isomorphic space R' as

$$T'_g = WT_gW^{-1} \tag{1.66}$$

It is easily verified (eq. (1.8)) that this equation defines a representation of G in space R'. Inversely,

$$T_g = W^{-1}T'_gW \tag{1.67}$$

Representations $\{T_g\}$ and $\{T'_g\}$ are called *equivalent*. In applications, equivalent representations are completely interchangeable, and the choice between them is determined by their convenience for a particular space.[7]

Operator F_n defines an isomorphism between the subspace of wave functions R_n (the eigensubspace of energy H_0 associated with the eigenvalue E_n) and the subspace

7 If R and R' coincide, eq. (1.66) admits the following "passive" interpretation. Group G is represented by *matrices* T_g to determine operators on the space R in some chosen basis. When switching to another basis, these matrices are replaced by matrices T'_g (eq. (1.66)), where W is the transformation matrix of the basis. With this interpretation, T_g and T'_g represent the same operator in different bases. We make this remark so that the reader could compare our discussion with available textbooks on the representations of groups.

F_n (composed of four-dimensional spherical functions of order $(n-1)$). Now find the images of this isomorphism as a result of its action on the representations of three-dimensional rotations (eq. (1.9)). By definition of representation $\{T_O\}$, rotation O corresponds to the operator $T_O\psi = \psi'$, where $\psi'(x) = \psi(O^{-1}x)$. In the momentum representation, function $\psi(x)$ corresponds to $\widetilde{\psi}(p)$ (eq. (1.38)), and $\psi'(x)$ to $\widetilde{\psi}'(p)$. Then the operator T_O corresponds in the momentum space to the operator which carries $\widetilde{\psi}(p)$ into $\widetilde{\psi}'(p)$.

To find this operator, $\psi'(x)$ is substituted instead of $\psi(x)$ in eq. (1.38), and then we have

$$\widetilde{\psi}'(p) = (2\pi\hbar)^{-3/2}\int \psi'(x)e^{-ipx/\hbar}d^3x$$

Replacing $\psi'(x)$ by $\psi(O^{-1}x)$ and changing variables $O^{-1}x = x'$, obtained are $O^{-1}x = x'$, $px = pOx' = O(O^{-1}p)Ox' = O^{-1}px'$, since the rotation preserves the scalar product, and $d^3x = d^3x'$, from whence

$$\widetilde{\psi}'(p) = (2\pi\hbar)^{-3/2}\int \psi(x')e^{-iO^{-1}px'/\hbar}d^3x'.$$

But the integral on the right differs from the integral (1.38) only by the notation of the integration variables and by $O^{-1}p$ substituted instead of p

Thus,

$$\widetilde{\psi}'(p) = \widetilde{\psi}(O^{-1}p) \tag{1.68}$$

and functions $\widetilde{\psi}(p)$ are transformed under rotations in the same way as $\psi(x)$.

Now consider transform (1.46) and find out how the argument in the left side of ξ (defined by angles $\alpha, \vartheta, \varphi$) changes when $O^{-1}p$ is substituted on the right side instead of p (eq. (1.68)). As follows from eq. (1.55), it is enough to take function $\psi(x)$ from R_n; then $E = E_n$ and $p_0 = \sqrt{-2mE_n}$ (eq. (1.44)) can be considered constant. Furthermore, $|O^{-1}p|=|p|$, and, as is seen from eq. (1.45), T_O does not change ξ_4 ($\xi'_4 = \xi_4$) and ξ_1, ξ_2, ξ_3 are transformed by the same matrix O^{-1} as p_x, p_y, p_z; so we have

$$\begin{aligned}
\xi'_1 &= o^{-1}_{11}\xi_1 + o^{-1}_{12}\xi_2 + o^{-1}_{13}\xi_3\\
\xi'_2 &= o^{-1}_{21}\xi_1 + o^{-1}_{22}\xi_2 + o^{-1}_{23}\xi_3\\
\xi'_3 &= o^{-1}_{31}\xi_1 + o^{-1}_{32}\xi_2 + o^{-1}_{33}\xi_3\\
\xi'_4 &= \xi_4
\end{aligned} \tag{1.69}$$

Since the factor of $\widetilde{\psi}(p)$ in eq. (1.46) does not change, operator T_O corresponds in the Fock space to the operator carrying $\Psi(\xi)$ into $\Psi(\xi')$, where ξ' is defined by eq. (1.69). The transform eq. (1.69) is inverse to the special four-dimensional rotation with matrix

$$O_{(4)} = \begin{bmatrix} o_{11} & o_{12} & o_{13} & 0 \\ o_{21} & o_{22} & o_{23} & 0 \\ o_{31} & o_{32} & o_{33} & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \tag{1.70}$$

Thus, in view of the Fock equivalence, the operator T_O in space R corresponds to the operator carrying $\Psi(\xi)$ into

$$\Psi'(\xi) = \Psi(\xi') = \Psi(O_4^{-1}\xi) \tag{1.71}$$

But this is a special case of a *four-dimensional* rotation operator (eq. (1.60)) corresponding to a special matrix (eq. (1.70)). Rotations (1.70) preserve the coordinate ξ_4, that is, $\xi'_4 = \xi_4$. All such rotations constitute a subgroup of SO(4), and each of them corresponds to the third order orthogonal matrix in the left-top corner of eq. (1.70); due to this correspondence, the subgroup is isomorphic to SO(3) and will be denoted simply SO(3). Therefore, *Fock equivalence carries the representation (1.9) of group SO(3) in the Schrödinger space of wave functions into the representation of the same group on the Fock space obtained from eq. (1.60) for the special rotation O taken in the form (1.70).*

As will be shown in the next chapter, the action of some group on the state space of a quantum system has fundamental importance not only for the kinematic description of states but also for the dynamics of the system. If the action of SO(3) group is isomorphically translated to the Fock space, so that "hydrogen" electron states are imaged by functions $\Psi(\xi)$, we obtain an equivalent representation of the form (1.60), where O are special four-dimensional rotations constituting the subgroup (eq. (1.70)). But now, using the isomorphic model of the space state, we can extend this subgroup by simply taking group SO(4) and its representation (1.60) together with *all* four-dimensional rotations O. Due to isomorphism F, decomposition (1.33) corresponds to the decomposition of the Fock space in terms of *invariant subspaces* of SO(4):

$$\mathsf{F} = \mathsf{F}_1 \oplus \mathsf{F}_2 \oplus \cdots \oplus \mathsf{F}_n \oplus \cdots \tag{1.72}$$

Decomposition (1.34) corresponds to the decomposition of F_n in terms of *irreducible subspaces* of SO(3):

$$\mathsf{F}_n = \mathsf{F}_{n,0} \oplus \mathsf{F}_{n,1} \oplus \cdots \oplus \mathsf{F}_{n,n-1}, \tag{1.73}$$

where F_{nl} is the image of space R_{nl} under the isomorphism. Finally, since basic functions $\psi_{nlm}(x, y, z)$ are carried into $\Psi_{nlm}(\xi)$, decomposition (1.29) corresponds to the decomposition of function $\Psi(\xi)$ defined on the sphere S^3, in terms of four-dimensional spherical functions:

$$\Psi(\xi) = \sum_{n,l,m} c_{nlm} \Psi_{nlm}(\xi) \tag{1.74}$$

Subspaces F_n are invariant even for the whole group SO(4). Indeed, as aforementioned in Section 1.2, F_n consists of four-dimensional spherical functions Y_{n-1} of order

$(n-1)$ obtained from homogeneous harmonic polynomials u_{n-1} of the same order, if their values are taken on the sphere S^3. Similar to the three-dimensional case (Section 1.1), the four-dimensional Laplace operator is proved to commute with rotation operators (eq. (1.64)) and, therefore, these operators carry $u_{n-1}(\xi_1, \xi_2, \xi_3, \xi_4)$ into polynomials of the same kind, namely, homogeneous harmonic polynomials of $n-1$ degree. But this means that F_n is an invariant subspace of group SO(4). Moreover, these subspaces are *irreducible* for SO(4) (see Appendix B).

If basis vectors ψ_{nlm} in Table 1.1 are changed for corresponding vectors Ψ_{nlm}, the resulting table will image the basis of space F. The columns of the table show the subspace F_n $(n = 1, 2, \ldots)$, and the expanded group SO(4) interconnects all cells of each individual column because corresponding subspaces are irreducible for SO(4). If the same representation (1.64) is considered only for the rotations of subgroup SO(3) (ξ_4 being preserved), the resulting representation of SO(3) for $n > 1$ will not be irreducible on subspaces F_n since each them is decomposed into irreducible subspaces F_{nl} of SO(3) group imaged by the rectangles of Table 1.1 (eq. (1.73)). This process, when a set of operators from some group is reduced to a set of operators from its subgroup, is called a *reduction* of the representation to the subgroup. Since isomorphisms preserve dimensions, the irreducible representation of SO(4) on the space F_n has dimension n^2 and, after being reduced to the subgroup SO(3), is decomposed into irreducible representations with dimensions 1, 3, 5,…, $2n-1$ (eq. (1.35)).

The question arises as to weather group SO(4) can be further expanded to make the *whole* Fock space irreducible, that is, the operators of the expanded group connect all columns of Table 1.1. In fact, such expansion is possible and was first applied to the hydrogen atom by Abalkin and Manko (1965). It was a so-called *conformal* group[8] SO(4,2), first used by Dirac (1937) for other purposes.

Consider a six-dimensional space with coordinates $(\xi_1, \ldots, \xi_6)$, which have no physical meaning. Group SO(4,2) consists of all linear homogeneous transformations C,

$$\begin{aligned} \xi'_1 &= c_{11}\xi_1 + \cdots + c_{16}\xi_6 \\ &\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots \\ \xi'_6 &= c_{61}\xi_1 + \cdots + c_{66}\xi_6 \end{aligned} \tag{1.75}$$

having determinant +1 and preserving the form

$$\xi_1^2 + \xi_2^2 + \xi_3^2 + \xi_4^2 - \xi_5^2 - \xi_6^2, \tag{1.76}$$

That is,[9]

8 The name of this group is due to its original definition as a group of conformal (angle-preserving) transformations of the Minkowski space. We use the definition proposed by Dirac.

9 In fact, we will need only those transformations (1.75) which are close to the identity transformation. "Global" issues are discussed in Fet (1975).

$$\xi'^2_1+\xi'^2_2+\xi'^2_3+\xi'^2_4-\xi'^2_5-\xi'^2_6=\xi^2_1+\xi^2_2+\xi^2_3+\xi^2_4-\xi^2_5-\xi^2_6. \tag{1.77}$$

Designation SO(4, 2) reflects the structure of the form (1.76).

There is a subgroup of SO(4, 2) consisting of transformations to preserve ξ_5, ξ_6, that is, $\xi'_5 = \xi_5$, $\xi'_6 = \xi_6$, and from eq. (1.77), we have

$$\xi'^2_1+\xi'^2_2+\xi'^2_3+\xi'^2_4=\xi^2_1+\xi^2_2+\xi^2_3+\xi^2_4. \tag{1.78}$$

Identified with the coordinates of the four-dimensional Euclidean space, the first four coordinates ξ_α can be regarded as four-dimensional rotations with matrices:

$$C=\left[\begin{array}{ccc|cc} o_{11} & \cdots & o_{14} & & \\ \vdots & & \vdots & 0 & \\ o_{41} & \cdots & o_{44} & & \\ \hline & 0 & & 1 & 0 \\ & & & 0 & 1 \end{array}\right], \tag{1.79}$$

where $(o_{\alpha\beta})$ $(\alpha, \beta = 1,\ldots, 4)$ are the orthogonal matrices with determinant +1 (see details in Section 5.2). Therefore, SO(4,2) contains a subgroup which is isomorphic to SO(4) and thus denoted simply SO(4). There is already a representation (1.62) of this subgroup in the Fock space F. This representation can be expanded to the representation $\{T_C\}$ of the whole group SO(4,2) *in the same space*, it means that for all transforms C of this group, we can define operators T_C to act in F and to constitute its representation, so that for $C = 0$, operator T_C coincides with the above-defined operator T_O of four-dimensional rotations (eq. (1.62)). Furthermore, space F is *unitary* and *irreducible* for representation $\{T_C\}$ (which is therefore infinite-dimensional and indecomposable into finite-dimensional representations).

Such a representation is not easy to construct due to the fact that functions $\Psi(\xi_1, \xi_2, \xi_3, \xi_4)$ of space F depend on *four* variables in contrast to transforms (eq. (1.75)) depending on *six* variables, so methods such as eqs. (1.9) or (1.72) are not applicable here. We will solve the task in Chapter 5 with the help of Lie algebras to be introduced in Chapter 3. So far, we assume that such representation exists, and make some physical conclusions.

To do that, we will use the inverse Fock isomorphism F^{-1} and define an equivalent representation of groups SO(4,2) on the space R of Schrodinger wave functions. As a result, we obtain a representation with irreducible subspaces R_n (instead of F_n) on the subgroup SO(4), and a representation with irreducible subspaces R_{nl} (instead of F_{nl}) on even smaller subgroup SO(3) (Table 1.1). Group SO(3) commutes with the general spherically symmetric Hamiltonian H (1.27). Group SO(4), to the contrary, no longer commutes with H, but commutes with the Coulomb Hamiltonian H_0; in fact, each eigenspace of Coulomb Hamiltonian R_n is invariant with respect to SO(4); therefore, for any function ψ from R_n and any operator of a four-dimensional rotation $T_{O_{(4)}}$, we have $T_{O_{(4)}}H_0\psi = T_{O_{(4)}}(E_n\psi) = E_nT_{O_{(4)}}\psi = H_0(T_{O_{(4)}}\psi)$, and from eq. (1.32) $T_{O_{(4)}}H_0\psi = H_0T_{O_{(4)}}\psi$

for all ψ from R. But for the group SO(4,2), we can no longer find a Hamiltonian to commute with the group; since the *whole* space R is irreducible for this group, such Hamiltonian would have the whole R as its eigenspace with a single eigenvalue. For this hypothetical Hamiltonian H_*, we would have

$$H_*\psi = E\psi \tag{1.80}$$

Such an operator is sometimes called "constant." Since energy is accurate within a constant, we can introduce a term H_* in the Hamiltonian equation (1.27), so that H_* is greatly exceeding all values of H_0 (for example, it can be the rest energy mc^2 of the electron). Finally, we introduce another term H_2 which does not commute with SO(3); for example, the energy of interaction of an electron with a uniform magnetic field along z axis; we assume, following the consideration of the Zeeman effect, that this field is weak, so that H_2 is small compared to H_1. Then the Hamiltonian has the form

$$H = H_* + H_0 + H_1 + H_2, \tag{1.81}$$

where H_* commutes with SO(4,2), H_0 commutes with SO(4), and H_1 commutes with SO(3). Hamiltonian equation (1.81) can be considered as consisting of a sequence of "perturbations," so that each of them is smaller than the preceding one. The largest member H_* corresponds to the system with the "highest symmetry" defined by group SO(4,2); perturbation H_0 reduces the symmetry, so that $H_* + H_0$ has the symmetry of subgroup SO(4); then the following perturbation H_1 reduces the symmetry to the subgroup SO(3). The last term H_2 completely breaks the symmetry of the system.[10]

Hamiltonians with a "step-like" structure of successively decreasing terms are very common in physics, perhaps, because only such operators in many cases allow solving the tasks of quantum mechanics with the methods of perturbation theory. In any case, the successive "*symmetry breaking*" is important for quantum mechanics and particularly for the applications we are interested in. We demonstrated the approach on the conventional example of the atomic electron. Successive symmetry reduction is described in this case by a nested chain of groups:

$$\mathrm{SO}(4,2) \supset \mathrm{SO}(4) \supset \mathrm{SO}(3) \tag{1.82}$$

Note also that the chain (1.82) corresponds to a special basis constructed above in the representation space $\Psi_{nlm}(\xi)$ (or, in its isomorphic space, $\psi_{nlm}(x)$). All vectors of the basis with a given n generate an irreducible subspace F of subgroup SO(4) ($n = 1, 2,\ldots$); all vectors with given n, l generate an irreducible subspace $\mathsf{F}_{nl} \subset \mathsf{F}_n$ of subgroup SO(3)($l = 0, 1,\ldots, n-1$); finally, the third index m, for given n, l enumerates individual

10 We do not take into account the rotational symmetry about z axis; this symmetry is useless, because after H_2 is added, we obtain an operator with *nondegenerate* eigenvalues, whose eigensubspaces are *one-dimensional* and not interesting as far as symmetry groups are considered.

basis vectors in $\mathsf{F}_{nl}(m = -l, -l+1, \ldots, l-1, l)$. As we will see, the numbers n, l, m can be obtained directly from the chain (1.82) without resorting to the Hamiltonian; they are called *quantum numbers* of the broken symmetry (1.82). Furthermore, the chain of groups makes it possible to construct a corresponding special basis without using the Hamiltonian and to classify the eigenstates; in more complex cases, this chain can help to guess the form of the Hamiltonian.

This chapter outlined the historical development of quantum mechanics. The equations of motion had the primary role, and groups were used only to solve and study them. The description of a quantum system was based on an energy operator, whose form is borrowed from the classical (nonquantum) physics in accordance with Bohr's "correspondence principle." Similarly, all other observables of a quantum system were obtained from classical observables by the "correspondence principle." The energy operator often happens to be symmetric, or, to put it mathematically, it commutes with some "symmetry group," or has a "step-like" structure of the terms with decreasing symmetry. From the Hamiltonian, a corresponding sequence of groups is constructed; irreducible representations of the symmetry group and its subgroups provide a kinematic description of the state space, a classification of states, and a numbering "quantum numbers" to indicate characteristic properties of the states and their place in the classification system.

There is also another approach, where the primary structure of physical reality is defined by a symmetry group or a chain of groups to express a successive "symmetry breaking" of the system. From the symmetry group, the observables or dynamic variables of the system are mathematically derived; they are used to construct a "step-like" Hamiltonian defining successive perturbations to express the given method of symmetry breaking. This approach was suggested by Wigner (1939) and is particularly useful in elementary particle theory which usually lacks a corresponding classical theory, and where the description of a system starts with guessing its symmetry.

In the next chapter, we will discuss these ideas and apply them to the description of the system of chemical elements.

2 Observables of a quantum system

2.1 Deriving observables from a symmetry group

According to the correspondence principle, each quantum system transforms in the "classical limit" into some corresponding classical system. For example, the electron in a central field corresponds to the classical system of a charge in a central field, considered as a particle of Newtonian mechanics. The Coulomb potential $1/r$, as a part of Schrödinger equation, was borrowed this way. In general, classical observables x, y, z correspond to the operators of multiplying ψ functions by x, y, z; and an arbitrary function $f(x, y, z)$ corresponds to the operator of multiplying by this function. Classical momenta $p_x = mv_x$, $p_y = mv_y$, $p_z = mv_z$ correspond to the operators of differentiating ψ functions with respect to coordinates $\frac{\hbar}{i}\frac{\partial}{\partial x}$, $\frac{\hbar}{i}\frac{\partial}{\partial y}$, $\frac{\hbar}{i}\frac{\partial}{\partial z}$, and the functions of p_x, p_y, p_z correspond to the same function of these operators: for example, the classical observable of kinetic energy $\frac{mv^2}{2} = \frac{1}{2m}(p_x^2 + p_y^2 + p_z^2)$ is associated with the same function of the momentum operator c. Thus, the classical expression of the electron's energy in a Coulomb field $\frac{mv^2}{2} - \frac{Ze^2}{r}$ generates a quantum Hamiltonian $H_0 = -\frac{\hbar^2}{2m} - \frac{Ze^2}{r}$ (eq. (1.36)). When the Hamiltonian is known, symmetry considerations sometimes facilitate the integration of the Schrödinger equation or the search of some qualitative properties of the energy spectrum. For example, the eigenfunctions and eigenvalues for a spherically symmetric Hamiltonian equation (1.56) may not always be possible to find, but if the dimensions of irreducible subspaces R_{nl} of group SO(3) are known, one can find the multiplicities of eigenvalues $2l + 1$. When a magnetic field is applied, spherical symmetry is broken and the energy level E_{nl} splits into $2l + 1$ nondegenerate levels, the same number as the dimension of the irreducible representation. Thus, traditional quantum mechanics considers symmetry groups as an applied tool to study dynamic equations obtained from the correspondence principle. Thus, the latter has the primary role in the construction of quantum mechanics, while the role of symmetry groups is, in a sense, secondary.

However, such method to obtain the observables works only for some simple quantum systems. For example, the spin of the electron cannot be derived this way as it has no classical analogy. Even less, the correspondence principle can be applied to quantum systems of the theory of elementary particles such as "isotopic multiplet" or "unitary multiplet" (e.g., "nucleon," "octet," and "decuplet"). To build such quantum-mechanical models, we need to use another method of guessing their symmetry groups and then obtaining from them the observables to describe the system, that is, a set of operators to acting on its state vectors. In this approach, the symmetry group is of primary importance, while the observables are derived from it.

Consider the method by the example from the nonrelativistic quantum mechanics of a single particle. Similar to the discussion in Section 1.1, we consider functions $\psi(x, y, z)$ (disregarding the spin and time dependence) to be state vectors of the system. In Section 1.1, we examined how SO(3) group acts on the

wave functions. Now we extend this group by introducing the group of motions or *isometry group* $M(3)$ composed of all nonhomogeneous linear transforms of the Euclidean space,

$$x' = Ox + a, \tag{2.1}$$

where O is the proper rotation $(\det|O| = +1)$, and a is the translation vector. Each movement can be obtained by consecutive rotation O and translation $Dx' = x + a$:

$$M = DO \tag{2.2}$$

A motion can be defined geometrically as the most general transform of the Euclidean space to preserve distances. In coordinates (eq. (2.1)), it has the form

$$\begin{aligned} x' &= o_{11}x + o_{12}y + o_{13}z + a_x \\ y' &= o_{21}x + o_{22}y + o_{23}z + a_y \\ z' &= o_{31}x + o_{32}y + o_{33}z + a_z \end{aligned} \tag{2.3}$$

A representation of the isometry group in the space of state vectors R can now be defined similar to the rotation group (see eq. (1.9)):

$$T_M\psi = \psi', \text{ where } \psi'(x) = \psi(M^{-1}x) \tag{2.4}$$

It is easily verified that eq. (2.4) is actually a representation, that is, the conditions in eq. (1.18) are fulfilled. The inverse transform M^{-1} in eq. (2.4) can be found if x, y, z in eq. (2.3) are expressed in terms of x', y', z':

$$\begin{aligned} x &= o_{11}^{-1}(x' - a_x) + o_{12}^{-1}(y' - a_y) + o_{13}^{-1}(z' - a_z) \\ y &= o_{21}^{-1}(x' - a_x) + o_{22}^{-1}(y' - a_y) + o_{23}^{-1}(z' - a_z) \\ y &= o_{31}^{-1}(x' - a_x) + o_{32}^{-1}(y' - a_y) + o_{33}^{-1}(z' - a_z) \end{aligned} \tag{2.5}$$

or

$$x = O^{-1}(x' - a) \tag{2.6}$$

Thus, the transformed function ψ' is written as

$$\begin{aligned} \psi'(x, y, z) = \psi(&o_{11}^{-1}(x - a_x) + o_{12}^{-1}(y - a_y) + o_{13}^{-1}(z - a_z), \\ &o_{21}^{-1}(x - a_x) + o_{22}^{-1}(y - a_y) + o_{23}^{-1}(z - a_z), \\ &o_{31}^{-1}(x - a_x) + o_{32}^{-1}(y - a_y) + o_{33}^{-1}(z - a_z) \end{aligned} \tag{2.7}$$

The isometry group $M(3)$ contains a subgroup of rotations SO(3) obtained for $a = 0$, and a subgroup of translations $D(3)$ obtained for $O = 1$. Its simplest subgroups are *one-parameter subgroups* whose elements M_α are parametrized by a continuous parameter α, so that the multiplication of these elements corresponds to the summation of the parameters:

$$M_{\alpha_1} M_{\alpha_2} = M_{\alpha_1+\alpha_2} \tag{2.8}$$

For example, consider a subgroup of translations along axis x. Designating the translation upon α as M_α, we have

$$M_\alpha(x, y, z) = (x + \alpha, y, z) \tag{2.9}$$

and the condition in eq. (2.8) is easily verified, because consecutive translations α_1 and α_2 are a single translation $\alpha_1 + \alpha_2$. Similarly, one-parameter subgroups of translations along y, z, or any axis are defined.

As another example, consider a subgroup of rotations about axis z. Designating the rotation by angle α as M_α, obtain

$$M_\alpha(x, y, z) = (x\cos\alpha - y\sin\alpha, x\sin\alpha + y\cos\alpha, z) \tag{2.10}$$

The condition in eq. (2.8) is also easily verified: consecutive rotations by angles α_1 and α_2 are the same as a single rotation by angle $\alpha_1 + \alpha_2$ (the angles with the difference 2π correspond to the same rotation). Similarly, one-parameter subgroups of rotations about y, z, or any arbitrary axis are defined.

In particular, representation $\{T_M\}$ of the isometry group defines the representations of its one-parameter subgroups. For the translations along x axis, we have

$$\psi_\alpha(x, y, z) = T_{M_\alpha}\psi(x, y, z) = \psi(x - \alpha, y, z) \tag{2.11}$$

(negative sign is due to M_α^{-1} under the function, see eq. (2.1)). The rate of change of ψ along some one-parameter subgroup is measured by its derivative with respect to α; the "initial rate" is

$$\frac{d}{d\alpha}\psi_\alpha(x, y, z)\big|_{\alpha=0} = \frac{d}{d\alpha}\psi(x - \alpha, y, z)\big|_{\alpha=0} = -\frac{\partial\psi(x, y, z)}{\partial x} \tag{2.12}$$

or, accurate within the sign, the operator of differentiation with respect to x. Quantum mechanics often operates with Hermitian operators since they have *real* eigenvalues; to obtain a Hermitian operator from eq. (2.12), we need only to multiply it by i. Finally, if a *momentum* operator is to be obtained, the desired dimension is achieved by factor $\hbar$ to result in operator p_x. For p_y and p_z, we have

$$p_x = \frac{\hbar}{i}\frac{\partial}{\partial x}, p_y = \frac{\hbar}{i}\frac{\partial}{\partial y}, p_z = \frac{\hbar}{i}\frac{\partial}{\partial z} \tag{2.13}$$

Similarly, for the rotations about z axis,

$$\psi_\alpha(x, y, z) = T_{M_\alpha}\psi(x, y, z) = \psi(x\cos\alpha + y\sin\alpha, -x\sin\alpha + y\cos\alpha, z) \tag{2.14}$$

The "initial rate" of change of ψ along some one-parameter subgroup is

$$\frac{d}{d\alpha}\psi_\alpha(x,y,z)|_{\alpha=0} = \frac{d}{d\alpha}\psi(x\cos\alpha + y\sin\alpha, -x\sin\alpha + y\cos\alpha, z)|_{\alpha=0}$$
$$= \frac{\partial\psi(x,y,z)}{\partial x}y - \frac{\partial\psi(x,y,z)}{\partial y}x = -\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)\psi(x,y,z) \quad (2.15)$$

Multiplying operator eq. (2.8) by $i\hbar$, obtain a Hermitian operator L_z having the dimension of the angular momentum. For L_x and L_y,

$$L_x = \frac{\hbar}{i}\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right),\ L_y = \frac{\hbar}{i}\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right),\ L_z = \frac{\hbar}{i}\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) \quad (2.16)$$

The situation is more complicated with the operators of coordinates which are relativistic and are associated with the Lorentz group. Without assuming any knowledge of relativistic quantum mechanics, we now show with simple reasoning that all observables of quantum mechanics are of "group origin." In relativistic mechanics, spatial and temporal coordinates are not considered separately, since they both change together with the coordinate system. Therefore, the state vector is a function of *four* variables $\psi(x, y, z, t)$ and describes also the temporal evolution of the system.[11] Instead of the rotation group, relativistic theory uses the *Lorentz group*; that is, the group of homogeneous linear transformations of variables x, y, z, t to preserve the form $x^2 + y^2 + z^2 - c^2t^2$. Denote the Lorentz transformation Λ, $x_1 = x$, $x_2 = y$, $x_3 = z$, $x_0 = ct$, and the point of space-time (x_1, x_2, x_3, x_0) as x. Similar to the motions in the Euclidean space, define "inhomogeneous Lorentz transformations" $x' = \Lambda x + a$, where a is the four-vector (a_1, a_2, a_3, a_0). This group is called the *Poincare group*; it contains (for $a = 0$) the Lorentz subgroup and (for $\Lambda = 1$) the subgroup of four-dimensional translations. In the space of wave functions Ψ, a representation of the Poincare group is defined similar to those of the rotation group (eq. (1.9)) and the isometry group (eq. (2.4)); that is, the Poincare transform $x' = p_x = \Lambda x + a$ is associated with the operator:

$$T_p\Psi = \Psi', \text{ where } \Psi'(x) = \Psi(P^{-1}x) = \Psi(\Lambda^{-1}(x - a)) \quad (2.17)$$

All observables of relativistic quantum mechanics are derived from one-parameter subgroups of the Poincaré group (except the spin observables to be discussed later).

One-parameter subgroups of translations along axes $x_\alpha(\alpha = 1, 2, 3, 0)$ are defined similar to that of eq. (2.9). The first three of them generate momentum operators p_1, p_2, p_3, and the fourth generates the operator:

$$\frac{d}{d\alpha}\Psi(x, y, z, x_0 - \alpha)|_{\alpha=0} = -\frac{\partial\Psi}{\partial x_0} = -\frac{1}{c}\frac{\partial\Psi}{\partial t}. \quad (2.18)$$

11 In fact, relativistic interpretation of the electron is impossible without considering the spin. So, the one-component wave function can refer here only to mesons with zero spin; but this point is of no importance for our goal of revealing the group origin of observables.

Thus, we obtain operator $\frac{\hbar}{i}\frac{\partial}{\partial x_0}$ similar to momentum operators, and after multiplying by $-c$, obtain the *energy operator*[12]

$$H = i\hbar\frac{\partial}{\partial t}. \tag{2.19}$$

Eigenfunctions of operator (eq. (2.9)), that is, wavefunctions with a definite value of (relativistic) energy E_r, have the form

$$\Psi(x) = e^{-iE_r t/\hbar}\chi(x, y, z). \tag{2.20}$$

If the particle is required to be at rest, that is, $\Psi = \Psi_0$ be an eigenfunction of p_1, p_2, p_3 with zero eigenvalues, we find $\chi = const$, then the energy E_r is the rest energy mc^2, and

$$\Psi_0(x) = e^{-imc^2 t/\hbar} \tag{2.21}$$

up to a constant factor.

For the case of a nonrelativistic limit, define *nonrelativistic* energy E by subtracting the rest energy from E_r. Writing the wave function as

$$\Psi(x) = e^{-imc^2 t/\hbar}\psi(x, y, z, t) \tag{2.22}$$

we see that

$$H\Psi = mc^2\Psi + e^{-imc^2 t/\hbar}H\psi \tag{2.23}$$

If ψ is an eigenfunction of H, then from eq. (2.23), the corresponding eigenvalue is E. For $E \ll mc^2$, we can therefore consider ψ as a nonrelativistic wave function with nonrelativistic energy E. Since any nonrelativistic wave function is expanded in a series in terms of eigenfunctions of the energy, we can generally interpret eq. (4.2) as an equation to connect, in the nonrelativistic limit, a relativistic wave function $\Psi(x)$ with the corresponding nonrelativistic wave function $\psi(x)$.

Consider now one-parameter subgroups generating the operators of angular momentum. The subgroup of rotations in the plane (x_1, x_2) has the form

$$\begin{aligned} x_1' &= x_1\cos\alpha - x_2\sin\alpha \\ x_2' &= x_1\sin\alpha + x_2\cos\alpha \\ x_3' &= x_3 \\ x_0' &= x_0 \end{aligned} \tag{2.24}$$

12 Multiplication by c gives the desired dimension, and the sign is chosen according to tradition. Note that the resulting operator stands on the left side of the nonrelativistic Schrödinger equation. From this point of view, Schrödinger equation is a relation between four-momentum operators p_α. A polynomial $p^2/2m$ of p_1, p_2, p_3 is also called the *energy operator*. From the Schrödinger equation, it follows that these two operators coincide for a wavefunction of motion in a real space.

and, since it preserves x_0, it coincides with the subgroup of rotations about axis z in a three-dimensional space. This subgroup generates the angular momentum operator

$$L_{12}\Psi = \frac{\hbar}{i}\left(x_1\frac{\partial}{\partial x_2} - x_2\frac{\partial}{\partial x_1}\right)\Psi, \tag{2.25}$$

which is quite similar to operator L_z (see eq. (2.16)). The same way obtain operators L_{23}, L_{31} from one-parameter subgroups of rotations in the planes (x_2x_3) and (x_3x_1); operators $L_{ik}(i, k = 1, 2, 3)$ play the role of operators of *spatial angular momentum* in the relativistic theory.

Finally, consider one-parameter subgroups of proper Lorentz transformations. In the plane (x_1x_0), such subgroup has the following form:

$$\begin{aligned} x_1' &= x_1 ch\alpha - x_0 sh\alpha \\ x_2' &= x_2 \\ x_3' &= x_3 \\ x_0' &= x_1 sh\alpha + x_0 ch\alpha \end{aligned} \tag{2.26}$$

where α and $\beta = v/c$ are connected by equations as

$$ch\alpha = (1-\beta^2)^{-1/2}, \quad sh\alpha = \beta(1-\beta^2)^{-1/2}. \tag{2.27}$$

So, eq. (2.26) coincides with the usual form of Lorentz transformations:

$$x' = \frac{x - vt}{\sqrt{1-(v^2/c^2)}}, \quad t' = \frac{t - \dfrac{v}{c^2}x}{\sqrt{1-(v^2/c^2)}}. \tag{2.28}$$

In the representation (2.17), this subgroup is associated with the generating operator:

$$\frac{d}{d\alpha}\psi(x_1 ch\alpha - x_0 sh\alpha, x_2, x_3, -x_1 sh\alpha + x_0 ch\alpha)\,|_{\alpha=0} = \left(-x_0\frac{\partial}{\partial x_1} - x_1\frac{\partial}{\partial x_0}\right)\psi. \tag{2.29}$$

Denote this operator, multiplied by $i\hbar$, as L_{01}. Similarly, construct operators L_{02} and L_{03} corresponding to proper Lorentz transformations in the planes (x_0x_2) and (x_0x_3), respectively. Operators

$$L_{0k} = \frac{\hbar}{i}\left(x_0\frac{\partial}{\partial x_k} + x_k\frac{\partial}{\partial x_0}\right) \tag{2.30}$$

are called *relativistic angular momenta*. For a particle having no spin, operators p_α and $L_{\alpha\beta}(\alpha, \beta = 1, 2, 3, 0)$ constitute a *complete set of observables in relativistic quantum mechanics*. Thus, the observables are obtained by a uniform way, namely,

they are operators which generate one-parameter subgroups of the main symmetry group.[13]

Now, we can explain the group origin of operators of multiplication by the coordinates in nonrelativistic quantum mechanics.[14] Apply operator L_{01} to the wave function Ψ in the form of eq. (2.22):

$$\begin{aligned} L_{01}\Psi(x) &= \frac{\hbar}{i}\left(x_0\frac{\partial}{\partial x_1} + x_1\frac{\partial}{\partial x_0}\right)\Psi(x) = \frac{\hbar}{i}\left(ct\frac{\partial}{\partial x} + \frac{x}{c}\frac{\partial}{\partial t}\right)e^{-imc^2t/\hbar}\psi(x,y,z,t) \\ &= \frac{\hbar}{i}e^{-imc^2t/\hbar}\left[ct\frac{\partial\psi}{\partial x} + \frac{x}{c}\left(-\frac{imc^2}{\hbar}\psi + \frac{\partial\psi}{\partial t}\right)\right] \\ &= e^{-imc^2t/\hbar}\left[ct\frac{\hbar}{i}\frac{\partial\psi}{\partial x} - \frac{x}{c}\left(mc^2\psi + i\hbar\frac{\partial\psi}{\partial t}\right)\right] \end{aligned} \tag{2.31}$$

Operators in the parentheses on the right-hand side of the equation have different values in the nonrelativistic approximation. The second of them, $i\hbar\frac{\partial}{\partial t}$, is the operator of *nonrelativistic energy* (since it is applied to nonrelativistic ψ); by assumption, its matrix elements are small compared to mc^2; therefore, the operator can be neglected. The resulting operator should be considered at a fixed moment of time, because in nonrelativistic case, state vectors are functions of x, y, z and contain t as a parameter only, so observables do not depend on t.[15] Then eq. (2.31) is a linear combination of p_x and the operator of multiplication by x. Since the first is constructed from the Poincare group, the second can also be explained in terms of a group theory.

In nonrelativistic quantum mechanics, there are some difficulties when deducing observables from a symmetry group. Full-symmetry group in nonrelativistic quantum mechanics is the *Galilean group* generated by rotations, translations, and proper Galilean transforms defining a uniform and rectilinear motion system at rate v:

$$x' = x + vt \tag{2.32}$$

This group has poor algebraic properties which makes it difficult to build its representations. Apparently, it relates to some formal imperfection of nonrelativistic mechanics capable to describe only slow motions.

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13 Later we will show that other observables are obtained as functions of those described above.

14 Note that *relativistic* quantum mechanics does not contain operators of multiplication by coordinates which are obtained, as we will see, in the *nonrelativistic limit* from the operators of relativistic angular momentum (eq. (2.30)).

15 Here, we discuss the so-called "Schrodinger representation." In the "Heisenberg representation," state vectors, in contrast to observables, are time-independent.

2.2 Quantum numbers of symmetry groups and their physical meaning

As shown above, observables of a quantum system can be derived from its symmetry group. Of course, the choice of the observables is not unique: for example, the operators of momentum and angular momentum derived from the isometry group depend on coordinate axes, and, therefore, on one-parameter subgroups. However, it will be shown that the number of such linearly independent observables depends on the group only. All observables are Hermitian operators, which act on the space of state vectors of a quantum system. As is known, for the set consisting of the maximum number of commuting operators, there are common eigenvectors which can be numbered by corresponding sets of eigenvalues. The eigenvalues used for such numbering are called *quantum numbers* of the symmetry group.

Consider, for example, the action of the isometry group $M(3)$ on the space R of Schrodinger wave functions $\psi(x, y, z)$ (eq. (2.4)). This group generates the operators of momentum p_x, p_y, p_z and angular momentum L_x, L_y, L_z. As is easily verified, momentum operators commute with each other but do not commute with angular momentum operators, and also angular momentum operators do not commute with each other. The maximum number of commuting operators is three: p_x, p_y, p_z. Common eigenfunctions of these operators are plane waves:

$$\psi_{q_x q_y q_z}(x, y, z) = e^{i(qx)/\hbar} = e^{i(q_x x + q_y y + q_z z)/\hbar}. \tag{2.33}$$

Function (2.33) corresponds to eigenvalues q_x, q_y, q_z of operators p_x, p_y, p_z. Since functions (2.33) are not square-integrable (eq. (2.1)), they do not belong to the Hilbert space R and hence are not wavefunctions in the strict sense of the word. There exist no infinite wave packets (eq. (2.33)) in nature: each wave packet is a plane wave in some limited area and vanishes at infinity. However, in theoretical studies, it is useful to consider also "nonnormable" wavefunctions; furthermore, plane waves are particularly important and the very term "wave function" originates from them. Eigenvalues q_x, q_y, q_z change continuously ("belong to a continuous spectrum") and take any real values. Since any wave function can be expanded in a Fourier integral (eq. (1.38)), that is, in a "continuous linear combination" of plane waves, functions (eq. (2.33)) form a (continuous) basis of space R for all possible sets of quantum numbers (q_x, q_y, q_z).

As a second example, consider the rotation group SO(3) in space R. The observables of the group are L_x, L_y, L_z; the maximum system of commuting observables contains only one of them, for example, L_z. Space R can be decomposed into a sum of irreducible subspaces of group SO(3); one way to do this was discussed in Section 1.1, where irreducible subspaces are denoted as R_{nl}. Each of them has the basis $\psi_{nlm}(x, y, z) = f_n(r)Y_l^{(m)}(\vartheta, \varphi)$ (eq. (1.28)) composed of eigenfunctions of operator L_z with eigenvalues $m = -l, -l+1, \ldots, l-1, l$. In contrast to the previous example, the quantum

number of the group SO(3) (single, in this specific case) is insufficient to number the basis of the *entire* R: it enumerates only the basis for each *irreducible* subspace. Later, we will obtain from symmetry groups two other quantum numbers l and n.

Some observables in quantum mechanics such as the operator of kinetic energy

$$E_{\text{кин}} = \frac{1}{2m}(p_x^2 + p_y^2 + p_z^2) \tag{2.34}$$

and the operator of total angular momentum[16]

$$L^2 = L_x^2 + L_y^2 + L_z^2 \tag{2.35}$$

cannot be obtained from a symmetry group with the above method.

However, all known observables are *functions* of those obtained from one-parameter subgroups of the symmetry group. We will call the latter *main observables* of the symmetry group, and the Hermitian operators which are functions of the main observables, we will call simply *observables*. Equations (2.34) and (2.35) are the quadratic functions of the main observables of the isometry group.

Casimir operators of the symmetry group are polynomials of main observables commuting with all of them. Operator (2.34) commutes with all momenta and angular momenta and, therefore, is a Casimir operator of the isometry group. As we will see, Casimir operator of G commutes also with all operators T_g; this implies that the Laplace operator (different from E_{kin} only by factor $2m$) commutes with the operators of translation and rotation. This explains the role of Laplace operator in mathematical physics. Operator (2.35) commutes with all momenta and, therefore, is a Casimir operator of rotation group; therefore, it also commutes with all operators of rotation T_O.

The following theorem of representation theory, the so-called "Schur's lemma," formulates the most important property of Casimir operators[17]:

All vectors of an irreducible space of a group are eigenvectors of its Casimir operator having the same eigenvalue. In other words, irreducible space of a group is an eigenspace of its Casimir operator C; that is, for all vectors, ψ of such space $C\psi = \lambda\psi$ for some λ. Therefore, operator C is *constant* on the space of the irreducible representation and has value λ. Schur's lemma will be proved in Chapter 3, and here, we illustrate it with some examples.

Irreducible subspaces of the isometry group are defined in R as those where H_{kin} is constant, since H_{kin} is the Casimir operator of the isometry group:

16 Designation L^2 should be understood as a single sign for the operator on the right side of eq. (2.35). Usually, operator L (root of L^2) is not considered.

17 The theorem was proved by I. Schur and the term "lemma" is a purely historical confusion.

$$\frac{1}{2m}(p_x^2 + p_y^2 + p_z^2)\psi = E\psi \quad \text{or} \quad -\frac{\hbar^2}{2m}\Delta\psi = E\psi \tag{2.36}$$

This is a Schrödinger equation for stationary states of a free particle. Thus, the value of the Casimir operator H_{kin} on an irreducible subspace of the isometry group is the energy of a free particle.

Irreducible subspaces of the rotation group (eq. (2.35)) are defined in R as those where the operator of total angular momentum is constant:

$$L^2\psi = \lambda\psi. \tag{2.37}$$

It is known (see also Section 1 in Appendix B) that eigenvalues of this equation are $\lambda = l(l+1)\hbar^2$, where $l = 0, 1, 2, \ldots$ In particular, on the subspace R_{nl}, the values of L^2 are $l(l+1)\hbar^2$. Thus, on an irreducible subspace of the rotation group, the Casimir operator L^2 defines the maximum value l of the projection of the angular momentum L_z and the dimension $2l+1$ of the subspace. This suggests a group interpretation of number l. If we call quantum numbers also the eigenvalues of Casimir operators of the symmetry group and its subgroups, then $l(l+1)$ is a quantum number of group SO(3); it is determined by an integer number l which is often also called a quantum number. However, there is not an observable of group SO(3) with values l for the basis vectors: for $l \neq m$, number l does not coincide with the value m of L_z or with the value of any other observable of SO(3). We will distinguish "true" quantum numbers (eigenvalues of the observables) from the parameters to define them (like l defines $l(l+1)$).

The third index n is associated with the group SO(4) and numbers the eigenfunctions of an electron in the Coulomb field. By Fock transform, $\psi_{nlm}(x, y, z)$ is carried into $\Psi_{nlm}(\xi)$ defined on the sphere S^3, and the space R_n generated by eigenfunctions with given n is carried into the irreducible subspace F_n of SO(4). To find this subspace in F, we will use Casimir operator of SO(4) the same way as for the full angular momentum as in eq. (2.35):

$$\Lambda^2 = \sum_{\alpha,\beta=1}^{4} L_{\alpha\beta}^2 \tag{2.38}$$

where $L_{\alpha\beta}$ corresponds to the one-parameter rotation group in the plane $(\xi_\alpha \xi_\beta)$:

$$L_{\alpha\beta}\Psi = \frac{\hbar}{i}\left(\xi_\alpha \frac{\partial}{\partial \xi_\beta} - \xi_\beta \frac{\partial}{\partial \xi_\alpha}\right)\Psi. \tag{2.39}$$

To prove that Λ^2 commutes with all operators $L_{\gamma\delta}$ (e.g., L_{12}), represent Λ^2 as

$$\Lambda^2 = (L_{12}^2 + L_{23}^2 + L_{31}^2) + (L_{12}^2 + L_{24}^2 + L_{41}^2) - L_{12}^2. \tag{2.40}$$

Since first bracket in eq. (2.40) is L^2 and $L_{ik}(i, k = 1, 2, 3)$ have the same expressions as in the three-dimensional case (x, y, z replaced by ξ_1, ξ_2, ξ_3), then L_{12} commutes with the first bracket. The second bracket is obtained from the first only by substituting ξ_4

instead of ξ_3, so L_{12} commutes also with the second bracket. Since the degrees of the same operator commute, L_{12} commutes with $-L_{12}^2$ and Λ^2. So Λ^2 is the Casimir operator of SO(4).

Space F_{n+1} consists of n-th degree homogeneous harmonic polynomials of $\xi_1, \xi_2, \xi_3, \xi_4$. Since all such polynomials form an irreducible subspace of SO(4), by Schur's lemma, they are all eigenfunctions of Λ^2 with the same eigenvalue λ. To find λ, it is enough to take *one* polynomial u_n and calculate $\Lambda^2 u_n$. Take a polynomial that depends only on ξ_1, ξ_2: $u_n(\xi_1, \xi_2) = (\xi_1 + i\xi_2)^n$. Defining $\xi_1 + i\xi_2 = \zeta$ obtain that $\mathrm{Re}\zeta^n$ and $\mathrm{Im}\zeta^n$ are homogeneous polynomials of degree n, they are harmonic (since they are real and imaginary parts of analytic function ζ^n); therefore, ζ^n is also a harmonic function of ξ_1, ξ_2 (consequently, also of $(\xi_1, \xi_2, \xi_3, \xi_4)$). Accurate with designations, the first term of eq. (2.40) is L^2. Considering u_n as a polynomial of *three* variables ξ_1, ξ_2, ξ_3, we have $(L_{12}^2 + L_{23}^2 + L_{31}^2)u_n = n(n+1)\hbar^2 u_n$ (l being replaced by n). The second bracket takes the same value. Now find $L_{12}^2 u_n$. Introducing a polar angle φ in the plane (ξ_1, ξ_2), obtain $L_{12} = \frac{\hbar}{i}\frac{\partial}{\partial\varphi}$, $\zeta^n = e^{in\varphi}$, and $L_{12}^2 u_n = n^2\hbar^2 u_n$. So, $\Lambda^2 u_n = [2n(n+1) - n^2]\hbar^2 u_n = n(n+2)\hbar^2 u_n$. Replacing n by $n-1$, we obtain that the value of Λ^2 on the irreducible subspace F_n is $(n^2-1)\hbar^2$.

Thus, for the "hydrogen" electron, the indices n, l, and m of wavefunctions are associated with the group SO(4) and its subgroup SO(3). In the space of Schrodinger wave functions, $n^2 - 1$ is the value of the Casimir operator of group SO(4) on its irreducible subspace R_n, and $l(l+1)$ is the value of the Casimir operator of group SO(3) on its irreducible subspace $\mathsf{R}_{n,l}$; finally, m is the eigenvalue of the observable L_z of group SO(3). Indices ψ_{nlm} indicate, therefore, the position of the basis vector in the irreducible subspaces of the chain $\mathrm{SO}(4) \supset \mathrm{SO}(3)$. Though the numbers n, l have no direct meaning for the group SO(4), we will also call them quantum numbers due to their connection with Casimir operators.

As we will see, number n is an eigenvalue of one of the main observables of the SO(4,2) group.

3 Lie groups and Lie algebras

3.1 Lie groups

The groups mentioned in the previous chapter, such as rotation groups SO(3) and SO(4), the isometry group of three-dimensional Euclidean space $M(3)$, Lorentz and Poincare groups, conformal group SO(4,2) are important for Physics and share a common property of their elements being described by continuous parameters. Now we show, by example of SO(3) group, how these parameters can be set.

The elements of SO(3), or proper rotations, are defined in a fixed-coordinate system by orthogonal matrices of the third order $O = (o_{ij})$ with determinant +1. The elements of an orthogonal matrix are connected by six independent relations

$$\sum_{k=1}^{3} o_{ik}o_{jk} = \delta_{ij}(i, j = 1, 2, 3), \tag{3.1}$$

where $\delta_{ij} = 1$ for i = j and $\delta_{ij} = 0$ for $i \neq j$. The independence of these relations means that none of them is a consequence of the others (we will not prove it here); the elements of orthogonal matrix are also connected by other relations which can be obtained by interchanging the first and the second indices in eq. (3.1), but these relations depend on relations (eq. (3.1)) (namely, equivalent to them). Generally speaking, from six equations (eq. (3.1)), one can express six variables o_{ij} in terms of three others, which can vary independently and determine an orthogonal matrix. Therefore, SO(3) is a three-parameter group.

However, the procedure for solving the equations meets difficulties: when we said that it is possible "generally speaking," we had in mind the following limitations. First, it is required that the Jacobian of six functions in the left-hand side of eq. (3.1) be nonzero for any values $o^0_{ij}(i, j = 1,2,3)$ with respect to six selected variables o_{ij}; under this condition, six selected matrix elements can be expressed in terms of the three others $o_{i_1j_1}, o_{i_2j_2}, o_{i_3j_3}$ in a sufficiently small vicinity of values $o^0_{i_1j_1}, o^0_{i_2j_2}, o^0_{i_3j_3}$, where these three parameters can change freely. But this assumption is not always true. If, for example, for some matrix O^0, one of the three elements $o^0_{i_kj_k}$ equals unity, then these three elements cannot be *free parameters*, because from eq.(3.1), it follows that $|o_{ij}| \leq 1$ (for i = j). But then the corresponding Jacobian should go to zero with respect to six other elements and, therefore, the above procedure is not applicable. It can be verified that for any orthogonal matrix O^0, there are such six elements that the above Jacobian is nonzero; but, as was shown, they cannot be chosen with the same method for the *whole* group. Thus, the parameterization of group SO(3) with three matrix elements (o_{ij}) is *local*: we need to use different triples of elements to describe different parts of the group.

Euler angles provide a more intuitive parameterization of group SO(3). Let x, y, z be a right-handed coordinate system, which we call a "fixed" coordinate system

(Fig. 3.1), then a proper rotation O can be defined by introducing a "moving" right-handed coordinate system x', y', z' which is obtained from the "fixed" system by rotation O. The position of "moving" axes with respect to the "fixed" axes is defined as follows. Take the intersection line of planes (xy), $(x'y')$ ("nodal line") and choose a direction on it; let φ denotes the angle between this direction and the axis x. ψ denotes the angle in the plane $(x'y')$ between the positive direction of the nodal line and the axis x'. Finally, ϑ denotes the angle between axes z and z'. In Euler coordinates, the position of axes x', y', z' and, thereby, rotation O is described by angles $\varphi, \psi,$ *and* ϑ, where $0 \le \varphi \le 2\pi$, $0 \le \psi \le 2\pi$, and $0 \le \vartheta \le \pi$.

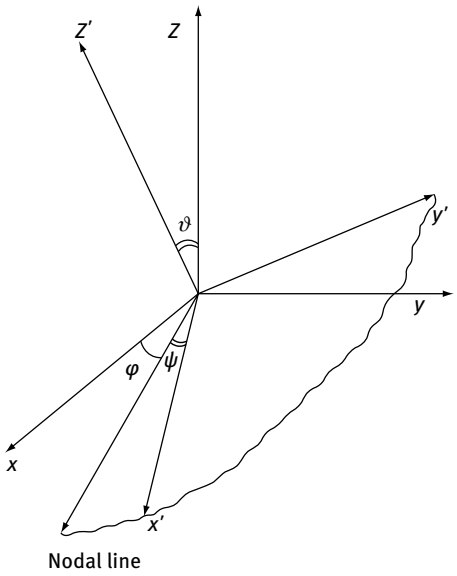


Fig. 3.1: Euler angle parameterization for SO(3) group.

The disadvantage of this parameterization is that it is not a one-to-one correspondence: values $\varphi = 0$, $\varphi = 2\pi$ and $\psi = 0$, $\psi = 2\pi$ correspond to the same rotation. Furthermore, the axis of rotation is not determined for the identical rotation, and the position of the nodal line is not defined for rotations about axis z, so that these rotations cannot be associated with no definite Euler angles. Therefore, Euler angles do not provide a one-to-one parameterization for the *whole* group SO(3). The same problem is met when longitude and latitude are defined on a two-dimensional sphere.

Wigner suggested an intuitive *local* parameterization of SO(3) (Wigner, 1959, p. 110). According to Euler's theorem (from the kinematics of rigid body), each non-identical rotation has a uniquely defined axis of rotation and can be obtained by rotation about this axis by an angle defined up to 2π. Let l be some axis and (l, w) a point on it at a distance $\frac{w}{\pi}$ from the origin ($w > 0$ stands for the direction of the axis

and $w < 0$ for the opposite direction). Point (l, w) will represent the rotation about axis l by (positive or negative) angle w. Small angles correspond to the points in the vicinity of the coordinate origin; it is therefore natural to assign the coordinate origin to the identity rotation. The points of a ball K with the radius exceeding unity, for example, $x^2 + y^2 + z^2 < 4$, represent all possible rotations, and points (l, w) and $(l, w + 2\pi)$ represent the same rotation. If K is covered by a finite number of areas ε_i such that none of them contains such pair of points, then in each ε_i, coordinates (x, y, z) determine a one-to-one continuous parameterization of some part of group SO(3), and each rotation belongs to one of these parts.

The above example shows that generally we cannot parametrize the *whole* group and are to content with local parameterization. The symmetry groups we will need, namely, *Lie groups*, allow good local parameterization. Lie groups are defined as follows:

Let G be a group. Suppose that G *contains a finite or infinite sequence of sets* $\varepsilon_1, \varepsilon_2, \ldots$ *which fully cover* G, *that is*,

(1) Each element *g* of G belongs to at least one of sets ε_i.
Suppose also that each set ε_i *allows parameterization in the sense that*

(2) For each ε_i, there is a region D_i of *n*-dimensional Euclidean space R^n which is in a one-to-one correspondence with ε_i. Each element g from ε_i is associated with coordinates $\alpha_1^{(i)}, \ldots, \alpha_n^{(i)}$ of its corresponding point in R^n interpreted as parameters. The same R^n with the same Cartesian coordinate system is taken for all *i*. The correspondence between ε_i and D_i defines *i*-th parameterization (in ε_i).
The parameterizations are connected as follows:

(3) If g belongs simultaneously to ε_i and ε_j and has, therefore, both *i*-th and *j*-th parameterizations, then parameters of g in these parameterizations $\alpha_1^{(i)}, \ldots, \alpha_n^{(i)}$ and $\alpha_1^{(j)}, \ldots, \alpha_n^{(j)}$ obey the equation,

$$\begin{aligned} \alpha_1^{(i)} &= f_1^{(ij)}(\alpha_1^{(j)}, \ldots, \alpha_n^{(j)}) \\ &\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots \\ \alpha_n^{(i)} &= f_n^{(ij)}(\alpha_1^{(j)}, \ldots, \alpha_n^{(j)}), \end{aligned} \tag{3.2}$$

where $f_n^{(ij)}$ are continuously differentiable functions of *n* arguments.

If the above requirements are satisfied, the group G is called a *Lie group*.

Evidently, this method of local parameterization is not unique: one and the same Lie group can be determined by different local parameters. It is only required that different parameterizations be related with each other via continuously differentiable maps. In other words, Lie group is not a group with a fixed system of local parameterization; rather, it is a group which *can* be parametrized "well enough," that is, by parameters changing in a continuously differentiable manner when *g* varies. The number of parameters *n* is called a *dimension* of the group and it does not depend on the chosen method of parameterization. Parameters α_k are quite similar to the curvilinear

coordinates in space or on a surface and sometimes we will refer to them as *local coordinates* on group G.

In the previous example (parameterization of SO(3)), the parameters in different sets ε_i are connected by equations $x^{(i)} = x^{(j)}$, $y^{(i)} = y^{(j)}$, $z^{(i)} = z^{(j)}$ or

$$\begin{aligned} x^i &= \left(1 - \frac{2}{\sqrt{(x^j)^2 + (y^j)^2 + (z^j)^2}}\right) x^j, \\ y^i &= \left(1 - \frac{2}{\sqrt{(x^j)^2 + (y^j)^2 + (z^j)^2}}\right) y^j, \\ z^i &= \left(1 - \frac{2}{\sqrt{(x^j)^2 + (y^j)^2 + (z^j)^2}}\right) z^j \end{aligned} \tag{3.3}$$

which can be verified by reader. If we take as parameters different triples of elements of orthogonal matrix o_{ij}, eq. (3.2) is obtained, as stated above, by solving eq. (3.1); the explicit expression of functions (3.2) is impossible in this case.

Exponential transform provides a standard parameterization of Lie groups easily used to discover their dimension. We apply it to the so-called *matrix* Lie groups, that is, homogeneous linear transformations of a finite-dimensional space represented by matrices in some coordinate system. The product of transformations corresponds to the product of the matrices, the identity transformation corresponds to the identity matrix, and the inverse transformation corresponds to the inverse matrix. All complex nondegenerate matrices of order n constitute a *general linear group* $\mathrm{GL}(n, C)$.[18] Any group of matrices of order n is a subgroup of $\mathrm{GL}(n, C)$ and is defined by certain relations. Thus, the orthogonal group of order n, $O(n)$, has *real* elements and its inverse matrices O^{-1} coincide with transposed matrices ${}^tO$ (eq. (3.1)):

$$\mathrm{Im}O = 0,\ O^{-1} = {}^tO,\ \text{ or } \mathrm{Im}o_{ij} = 0,\ o_{ij}^{-1} = o_{ji}. \tag{3.4}$$

The group of proper rotations $\mathrm{SO}(n)$ is obtained by additional requirement $\det|O| = 1$, the unitary group $U(n)$ by the condition that inversed matrices U^{-1} coincide with their transposed complex conjugates ${}^tU^*$:

$$U^{-1} = {}^tU^*, \text{ or } u_{ij}^{-1} = u_{ji}^* \tag{3.5}$$

$\mathrm{SU}(n)$ group is obtained by additional requirement $\det|U| = 1$.[19] Orthogonal and unitary groups are particularly important for physics. Equally important is the Lorentz group which is *pseudo-orthogonal*. Group $\mathrm{SO}(p,q)$ consists of real matrices of order $p + q$, which have determinant 1 and define linear homogeneous transformations of

18 Groupe linéaire (n specifies the dimension of the space, C is a complex number).
19 Spécial unitaire (fr.) (Special unitary).

$(p+q)$-dimensional space to preserve the form $\xi_1^2 + \cdots + \xi_p^2 - \xi_{p+1}^2 - \cdots - \xi_{p+q}^2$. SO(3,1) is a Lorentz group, while SO(4,2) is a conformal group. Here we will not discuss pseudo-orthogonality conditions in their general form, and later consider the conformal group in detail.

Define the *exponential function* of matrix X as

$$U = e^X = 1 + X + \frac{1}{2!}X^2 + \cdots + \frac{1}{n!}X^n + \cdots \tag{3.6}$$

It can be verified that eq. (3.6) converges for any matrix X (i.e. the element $s_{ij}^{(n)}$ of its partial sum $S^{(n)}$ converges to u_{ij} for all i, j) and defines a continuous one-to-one correspondence between matrices X sufficiently close to the zero matrix and matrices U sufficiently close to the identity matrix. Thus, X can be considered as the logarithm of U from the vicinity of the identity matrix. Without these restrictions, the correspondence between X and U is no more a one-to-one correspondence. As is known, the logarithm function is not uniquely determined for complex numbers; the same is true for matrices $e^{2\pi i \cdot 1} = e^0$, where O is the zero matrix and 1 is the identity matrix. But the "real logarithm" is not always unique even for real matrices, as is seen from the example of matrices,

$$X_1 = \begin{bmatrix} 0 & -\pi \\ \pi & 0 \end{bmatrix}, \quad X_2 = \begin{bmatrix} 0 & \pi \\ -\pi & 0 \end{bmatrix}, \tag{3.7}$$

for which $e_1^X = e_2^X = -1$.

If matrices X, Y commute, all their degrees also commute; therefore, similar to numbers,

$$e^{X+Y} = e^X e^Y, \text{ if } XY = YX \tag{3.8}$$

As matrix $-X$ commutes with X, we have, in particular, $e^0 = e^X \cdot e^{-X}$ and

$$(e^X)^{-1} = e^{-X}. \tag{3.9}$$

In addition, that the following equation can be proved:

$$\det|e^X| = e^{trX}, \tag{3.10}$$

where $tr\, X = \sum_{i=1}^n x_{ii}$ is the trace of X. From eq. (3.9), it follows that e^X is a nondegenerate matrix for all X and that $\det X = 1$ for all traceless matrices X ($tr\, X = 0$).

Suppose X is a real antisymmetric matrix, that is, $\mathrm{Im} x_{ij} = 0$, $x_{ij} = -x_{ji}$ ($ImX = 0$), (${}^tX = -X$). Then for $O = e^X$, the inverse matrix coincides with the transposed one:

$$O^{-1} = e^{-X} = e^{{}^tX} = {}^t(e^X) = {}^tO, \tag{3.11}$$

that is, O is orthogonal. As mentioned above, all orthogonal matrices sufficiently close to the identity matrix can be uniquely represented as e^X, where X is a sufficiently small matrix. From eq. (3.10), it follows that determinants of sufficiently small matrices X are close to the identity. But $\det|{}^tO| = \det|O|$, and from ${}^tOO = 1$, obtain $(\det|O|)^2 = 1$, $\det|O| = \pm 1$; therefore, for small X, we have $\det|O| = 1$ and O belongs to SO(n).

Thus, eq. (3.6) defines a continuous one-to-one correspondence between matrices SO(n) close to identity and antisymmetric matrices close to zero. The latter are much easily parametrized: matrix X can be parametrized by its elements above the diagonal (x_{ij}, $i < j$) which completely determine real antisymmetric matrices. The number of such x_{ij} is $\frac{n(n-1)}{2}$. As follows from eq. (3.6), the same parameters x_{ij} can be assigned to the orthogonal matrix $O = e^X$ and thus, they define a parameterization of some vicinity of identity in SO(n). Now we can parameterize also a vicinity of any rotation O_0 by associating all matrices O close to O_0 with matrices $O' = OO_0^{-1}$ close to identity. Since the latter are already parameterized, we can assign to matrix O the same parameter values as those describing the corresponding matrix O'. This method of "group translation" is applicable to all Lie groups and allows reducing parameterization of a vicinity of any element to parameterization of a vicinity of identity. Evidently, the dimension of SO(n) is $\frac{n(n-1)}{2}$.

Similarly is parameterized SU(n) group. As it was done for eq. (3.11), matrix $U = e^X$ is proved to be unitary if ${}^tX^* = -X$ (here we have to use eq. (3.5) instead of eq. (3.4)). Such matrices X are called *antihermitian*. Independent parameters are chosen as real and imaginary parts of $\frac{n(n-1)}{2}$ elements above the diagonal and imaginary parts of their diagonal elements. Consequently, the dimension of the unitary group is $n(n-1) + n = n^2$. The condition $\det|U| = 1$ is not automatically fulfilled in this case and follows from the additional condition $tr\ X = 0$ (eq. (3.10)). Due to this condition, only $n-1$ diagonal elements of matrix X are independent, and the n-th element is expressed in terms of the others, so that the dimension SU(n) is $n^2 - 1$. So, the dimensions of groups SU(2), SU(3), SU(4), SU(5), and SU(6) are 3, 8, 15, 24, and 35, respectively.

It can be shown that the dimension of pseudo-orthogonal group $SO(p, q)$ depends on the sum $p + q$ rather than on p,q (i.e. the number of pluses and minuses in the quadratic form to determine the group). Therefore, the dimension of Lorentz group SO (3,1) is six, similar to that of SO(4) group; the dimension of the conformal group SO(4,2) is the same as that of SO(6); that is, $\frac{6 \cdot 5}{2} = 15$.

Now consider nonmatrix groups.[20] The elements of Euclidean translations group $D(3)$ are defined by translation vectors a having three components a_x, a_y, a_z; thus, the group is three-dimensional. The elements of Euclidean isometry group $M(3)$ are defined by pairs (O, a), where O is the rotation and a is the translation vector. Rotations and translations depend on three parameters each, so the dimension of $M(3)$ is 6. The elements of the Poincare group are defined by pairs (Λ, a), where Λ is the Lorentz transformation depending on six parameters, and a is the four-dimensional translation vector depending on four components; therefore, the dimension of the Poincare group is 10.

20 All Lie groups considered in physics are isomorphic to some matrix groups, but these matrix groups are artificially constructed and are not directly related to the space where the group originally acts. As these spaces (e.g. Euclidean or Minkowski spaces) are important for Physics, we do not replace such groups as isometry group or Poincare group by isomorphic matrix groups.

Lie groups can be *compact* or *noncompact*, depending on their topological structure. Roughly speaking, the difference between them is the same as between a closed finite line segment $a \le x \le b$ and the whole line $-\infty \le x \le \infty$. It is known that no sequence of points can "go to infinity" on a segment, rather it accumulates at least in one point x_0, whereas on the infinite line, there exists a sequence that "goes to infinity" (e.g. $x_k = 1, 2, 3, \ldots$). More exactly, a sequence of points $\{x_k\}$ is called compact if it contains a subsequence $\{x_{k_l}\}$ converging to some point x_0 (a *finite* limit). A set is called compact if any sequence of its points is compact. A closed finite segment is compact (Bolzano-Weierstrass theorem), but the entire line is not compact.

The line is a simplest Lie group (with the operation of addition), whereas the segment is not even a group. In fact, compactness can be defined for other objects than groups, but we will consider Lie groups only. Let G be a Lie group, $\{g_k\}$ is a sequence of its elements, g_0 is an element of G. Then there is a set ε which contains g_0 and is parameterized by parameters $\alpha_1, \ldots, \alpha_n$; let parameters of g_0 be $\alpha_1^{(0)}, \ldots, \alpha_n^{(0)}$. Assume that all g_k belong to ε starting from some number and have in ε parameters $\alpha_1^{(k)}, \ldots, \alpha_n^{(k)}$, and $\lim_{k\to\infty} \alpha_l^{(k)} = \alpha_l^{(0)} (l = 1, \ldots, n)$. Then g_k is said to converge to g_0. It is easily verified that this definition is independent on the chosen set ε containing g_0 (if there is more than one such set). This definition of convergence in a Lie group shows how parameterization of a group can be used. In the case of a matrix group G, the elements of matrix U belonging to G are numbers u_{ij} having is a well-known definition of convergence. u_{ij} are expressed, by definition of a Lie group, as continuous functions of some number of independent parameters, and the convergence of u_{ij} follows from the convergence of the parameters; in other words, for a matrix group, convergence of elements $U^{(k)} \to U^{(0)}$ means convergence of $u_{ij}^{(k)} \to u_{ij}^{(0)}$ for all i, j. For the group of translations, the convergence of translations $a^{(k)} \to a^{(0)}$ means $a_x^{(k)} \to a_x^{(0)}$, $a_y^{(k)} \to a_y^{(0)}$, $a_z^{(k)} \to a_z^{(0)}$. For the isometry group, convergence $(O^{(k)}, a^{(k)}) \to (O^{(0)}, a^{(0)})$ means $O^{(k)} \to O^{(0)}$ and $a^{(k)} \to a^{(0)}$. A sequence of elements $\{g_k\}$ of a Lie group G is called *compact*, if it contains a subsequence $\{g_k\}$ converging to some element g_0 of the group. A Lie group is called *compact* if any sequence of its elements is compact.

It is easily verified that SO(3) is compact. Indeed, from the orthogonality condition (3.1), it follows that $|o_{ij}| \le 1$ for all i, j (it is sufficient to consider the sum of squares of the elements of any row). If $\{O^{(k)}\}$ is a sequence of orthogonal matrices, then due to *finiteness* of the sequences $\{o_{ij}^{(k)}\}$, $k = 1, 2, \ldots$, we can find a subsequence $\{O^{(k_l)}\}$ such that numbers $o_{ij}^{(k_l)}$ converge for all i,j; that is, matrices $O^{(k_l)}$ converge to some matrix $O^{(0)}$. Transition to limit in eq. (3.1) proves that $O^{(0)}$ is also orthogonal and its determinant is 1.

Translation group is noncompact. Indeed, translations $a = (a_x, a_y, a_z)$ are parametrized by numbers a_x, a_y, a_z; a sequence of translations $a^{(k)} = (k, 0, 0)$ cannot contain a converging subsequence $a^{(k_l)}$ since numbers k_l in this case would have a finite limit.

All groups $\mathrm{SO}(n)$, $\mathrm{SU}(n)$ are compact, because they consist of matrices with finite elements. Isometry group and Poincare group are noncompact because they contain the subgroup of translations. Lorentz group and conformal group are also noncompact.

3.2 Lie algebras

As we saw, *one-parameter subgroups* of Lie groups are particularly important in physics because they can be used to obtain observables. One-parameter subgroups are most convenient to study for *matrix* Lie groups. Matrix groups consist of nondegenerate matrices of a specified order with an operation of group multiplication, so that the identity matrix (denoted 1) plays the role of identity, and the inverse matrix plays the role of the inverse element. Orthogonal and unitary groups are matrix groups. All groups of matrices of order n are subgroups of the *general linear group*; that is, the group of all nondegenerated matrices of order n with complex elements $\mathrm{GL}(n, C)$.

Since matrices define operators in a finite space, matrix groups can also be considered as *operator* groups. In fact, consider n-dimensional complex space C^n with coordinates $z_1, \ldots, z_n$. The addition of vectors is defined in C^n as

$$(z_1, \ldots, z_n) + (w_1, \ldots, w_n) = (z_1 + w_1, \ldots, z_n + w_n), \tag{3.12}$$

the multiplication by complex numbers as

$$\lambda(z_1, \ldots, z_n) = (\lambda z_1, \ldots, \lambda z_n). \tag{3.13}$$

The scalar product in C^n is defined as

$$\langle z|w\rangle = \sum_{i=1}^{n} z_i^* w_i, \tag{3.14}$$

and is easily verified to have the following properties:

$$\langle z + v|w\rangle = \langle z|w\rangle + \langle v|w\rangle, \langle w|z + v\rangle = \langle w|z\rangle + \langle w|v\rangle \tag{3.15}$$

(additivity);

$$\langle z|\lambda w\rangle = \lambda\langle z|w\rangle \tag{3.16}$$

for all complex λ (homogeneity with respect to the second factor),

$$\langle \lambda z|w\rangle = \lambda^*\langle z|w\rangle \tag{3.17}$$

for all complex λ ("antihomogeneity" with respect to the first factor),

$$\langle z|z\rangle \geq 0; \quad \langle z|z\rangle > 0 \quad \text{for } z \neq 0 \tag{3.18}$$

(positive definiteness).

Equations (3.15) and (3.16) mean *linearity* of scalar product with respect to the second factor and *antilinearity* with respect to the first factor.

Matrix $U = (u_{ij})$ defines a *linear transformation* or (what is the same) a *linear operator* in C^n as

$$z_i' = \sum_{j=1}^{n} u_{ij} z_j (i = 1, \ldots, n) \tag{3.19}$$

or, briefly

$$z' = Uz. \tag{3.20}$$

As is easily seen, a product of matrices corresponds to the product of operators in the same order. Thus, matrix groups may be considered as operator groups. If matrices U are unitary, that is, $U^{-1} = {}^tU^*$, then operators are also unitary:

$$\begin{aligned}\langle Uz|Uw\rangle &= \sum_{i=1}^{n}(Uz)_i^*(Uw)_i = \sum_{i=1}^{n}\left(\sum_{k=1}^{n}u_{ik}z_k\right)^*\left(\sum_{l=1}^{n}u_{il}w_l\right) = \sum_{k,l=1}^{n}\left(\sum_{i=1}^{n}u_{ik}^*u_{il}\right)z_k^*w_l \\ &= \sum_{k,l=1}^{n}\delta_{kl}z_k^*w_l = \sum_{k=1}^{n}z_k^*w_k = \langle z|w\rangle\end{aligned} \tag{3.21}$$

A one-parameter subgroup $\{U_\alpha\}$ of a matrix group G, by definition, satisfies the condition,

$$U_{\alpha_1+\alpha_2} = U_{\alpha_1}U_{\alpha_2} \tag{3.22}$$

For $\alpha_1 = \alpha_2 = 0$, obtain $U_0 = U_0^2$, whence $U_0 = 1$. Matrix U_α can be shown to depend on α in a continuous and even differential way, that is, $(u_\alpha)_{ij}$ are differentiable functions of α. As we saw in Chapter 2, observables are obtained from representations of one-parameter subgroups by differentiating $U_\alpha\psi$ with respect to α for $\alpha = 0$. In the case of matrix groups, this procedure can be carried out within the *group itself*. Let

$$A = i\lim_{\alpha\to 0}\frac{U_\alpha - 1}{\alpha} = i\frac{dU_\alpha}{d\alpha}\Big|_{\alpha=0} \tag{3.23}$$

and call A a *generating matrix* or a *generator* of a one-parameter subgroup (eq. (3.13)).

Factor i is introduced here for the following reason. *Unitary* representations of groups are most important in physics; in particular, eq. (3.19) defines a unitary representation in C^n for a unitary group. If U_α are unitary operators, then for any vectors z, w, the equation $\langle U_\alpha z|U_\alpha w\rangle = \langle z|w\rangle$ is identical with respect to α. Differentiation with respect to α gives

$$\frac{d}{d\alpha}\langle U_\alpha z|U_\alpha w\rangle\Big|_{\alpha=0} = \left\langle \frac{dU_\alpha}{d\alpha}z\,\middle|\,U_\alpha w\right\rangle\Big|_{\alpha=0} + \left\langle U_\alpha z\,\middle|\,\frac{dU_\alpha}{d\alpha}w\right\rangle\Big|_{\alpha=0} \tag{3.24}$$

and since $U_0z = z$, $U_0w = w$, for the operator $X = \frac{dU_\alpha}{d\alpha}|_{\alpha=0}$, obtain the identity

$$\langle Xz|w\rangle = -\langle z|Xw\rangle \tag{3.25}$$

Or, in coordinate form

$$\sum_{i=1}^{n}\left(\sum_{j=1}^{n}x_{ij}z_j\right)^*w_i = -\sum_{j=1}^{n}z_j^*\left(\sum_{i=1}^{n}x_{ji}w_i\right) \tag{3.26}$$

that is, $x_{ij}^* = -x_{ji}$ or ${}^tX^* = -X$. Matrices satisfying this condition (or, equivalently, operators satisfying (eq. (3.25))) are called *antihermitian*. Antihermitian operators are not popular with physicists, as their eigenvalues are purely imaginary. When multiplied by i, they become *Hermitian* matrices $A = iX$, and their elements satisfy the conditions $a_{ij}^* = a_{ji}$, or $A^+ = A$, and the corresponding operator satisfies the identity

$$\langle Az|w\rangle = \langle z|Aw\rangle \tag{3.27}$$

Hermitian operators have *real* eigenvalues: if $Az = \lambda z$, then

$$\langle Az|z\rangle = \lambda^*\langle z|z\rangle, \langle z|Az\rangle = \lambda\langle z|z\rangle, \tag{3.28}$$

and from eq. (3.27), it follows $\lambda^* = \lambda$. This property makes the Hermitian operators convenient observables, because their eigenvalues can be identified with real values observed experimentally.[21]

Derive a differential equation for one-parameter subgroups of a matrix group. Assuming in eq. (3.22) $\alpha_1 = \alpha$, $\alpha_2 = \beta$, we find

$$\frac{dU_\alpha}{d\alpha} = \lim_{\beta\to 0}\frac{U_{\alpha+\beta} - U_\alpha}{\beta} = \lim_{\beta\to 0}\frac{U_\alpha U_\beta - U_\alpha}{\beta} = \lim_{\beta\to 0} U_\alpha\frac{U_\beta - 1}{\beta} = U_\alpha\lim_{\beta\to 0}\frac{U_\beta - 1}{\beta} = -iU_\alpha A \tag{3.29}$$

(note that if $U_{\alpha+\beta}$ is written as $U_\beta U_\alpha$, then we have $-iAU_\alpha$, so that U_α and A commute). Therefore,

$$\frac{dU_\alpha}{d\alpha} = -iAU_\alpha \tag{3.30}$$

The solution of this matrix differential equation is the same as in the numerical case: $U_\alpha = Ce^{-i\alpha A}$. Assuming $\alpha = 0$ and taking into account that $U_0 = 1$, obtain the general view of a one-parameter subgroup of a matrix group:

$$U_\alpha = e^{-i\alpha A} \tag{3.31}$$

Thus, from the generator A determined by eq. (3.23), we can uniquely reconstruct a one-parameter subgroup.

Consider as an example a subgroup of SO(3) consisting of all rotations about coordinate axes. For the rotation by angle α about axis z, we have an orthogonal matrix

$$O_\alpha = \begin{bmatrix} \cos\alpha & -\sin\alpha & 0 \\ \sin\alpha & \cos\alpha & 0 \\ 0 & 0 & 1 \end{bmatrix}. \tag{3.32}$$

21 In mathematical literature, operator $X = \frac{dU_\alpha}{d\alpha}|_{\alpha=0}$ is called a generator of a one-parameter subgroup $\{U_\alpha\}$; if U_α are unitary, then X is an antihermitian. As follows from $A = iX$, both recordings are equivalent.

The generator of subgroup $\{O_\alpha\}$ is

$$A_3 = i\frac{dO_\alpha}{d\alpha}\Big|_{\alpha=0} = i\begin{bmatrix} -\sin\alpha & -\cos\alpha & 0 \\ \cos\alpha & -\sin\alpha & 0 \\ 0 & 0 & 0 \end{bmatrix}_{\alpha=0} = \begin{bmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}. \tag{3.33}$$

Verifying eq. (3.31),

$$A_3^2 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad A_3^3 = A_3, \quad A_3^4 = A_3^2, \text{ etc.}, \tag{3.34}$$

whence it follows

$$\begin{aligned} e^{-i\alpha A_3} &= 1 + (-i\alpha)A_3 + \frac{1}{2!}(-i\alpha)^2 A_3^2 + \cdots = \left(1 - \frac{\alpha^2}{2!} + \frac{\alpha^4}{4!} - \cdots\right)A_3^2 \\ &\quad - i\left(\alpha - \frac{\alpha^3}{3!} + \frac{\alpha^5}{5!} - \cdots\right)A_3 + (1 - A_3^2) = A_3^2\cos\alpha - iA_3\sin\alpha + (1 - A_3^2) = O_\alpha. \end{aligned} \tag{3.35}$$

Similarly, obtain the generators of the one-parameter subgroup of rotations about axes x,y:

$$A_1 = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{bmatrix}, \quad A_2 = \begin{bmatrix} 0 & 0 & i \\ 0 & 0 & 0 \\ -i & 0 & 0 \end{bmatrix}, \quad A_3 = \begin{bmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}. \tag{3.36}$$

As might be expected, these matrices are Hermitian. The reader is advised to write down the matrix representing rotation about an arbitrary axis and to find the corresponding generator.

As a second example, consider one-parameter subgroups of SU(2) generated by Hermitian matrices

$$\tau_1 = \begin{bmatrix} 0 & \frac{1}{2} \\ \frac{1}{2} & 0 \end{bmatrix}, \quad \tau_2 = \begin{bmatrix} 0 & -\frac{i}{2} \\ \frac{i}{2} & 0 \end{bmatrix}, \quad \tau_3 = \begin{bmatrix} \frac{1}{2} & 0 \\ 0 & -\frac{1}{2} \end{bmatrix}. \tag{3.37}$$

These matrices are connected to well-known Pauli matrices $\sigma_k = 2\tau_k$ ($k = 1,2,3$) satisfying equations $\sigma_k^2 = 1$. Thus,

$$U_\alpha^{(k)} = e^{-i\alpha\tau_k} = e^{-\frac{i\alpha}{2}\sigma_k} = 1 + \left(-\frac{i\alpha}{2}\right)\sigma_k + \frac{1}{2!}\left(-\frac{i\alpha}{2}\right)^2\sigma_k^2 + \cdots = \cos\frac{\alpha}{2} - i\sigma_k\sin\frac{\alpha}{2},$$

$$U_\alpha^{(1)} = \begin{bmatrix} \cos\frac{\alpha}{2} & -i\sin\frac{\alpha}{2} \\ -i\sin\frac{\alpha}{2} & \cos\frac{\alpha}{2} \end{bmatrix}, \quad U_\alpha^{(2)} = \begin{bmatrix} \cos\frac{\alpha}{2} & -\sin\frac{\alpha}{2} \\ \sin\frac{\alpha}{2} & \cos\frac{\alpha}{2} \end{bmatrix}, \quad U_\alpha^{(3)} = \begin{bmatrix} e^{-\frac{i\alpha}{2}} & 0 \\ 0 & e^{\frac{i\alpha}{2}} \end{bmatrix}.$$

These matrices are easily verified to be unitary. The reader is encouraged to find the most general one-parameter subgroup of SU(2).

For one-parameter subgroups, one can define *operations* which again produce one-parameter subgroups. To do that, we will need the following concept. A *curve* in the space of matrices is a family of matrices $\{X_\alpha\}$ dependent on some parameter. This concept is similar to the curve $r(\alpha)$ in usual space or on the surface defined by radius vector as a function of some parameter. The dependence is assumed continuously differentiable, that is, the components $r(\alpha)$ are continuously differentiable functions of α. Similarly, for a matrix curve $\{X_\alpha\}$, matrix elements $(\mathrm{x}_\alpha)_{ij}$ are assumed continuously differentiable functions of α. By analogy with the tangent vector $r'(\alpha)$ at point $r(\alpha)$, we can determine a tangent vector X'_α at the point of a matrix curve X_α as matrix

$$\frac{dX_\alpha}{d\alpha} = \lim_{\beta\to 0} \frac{X_{\alpha+\beta} - X_\alpha}{\beta} \tag{3.39}$$

The elements of this matrix are $\frac{d(x_\alpha)_{ij}}{d\alpha}$. We say that matrix curves $\{X_\alpha\}$ and $\{Y_\alpha\}$ are *tangent at the identity*, if

$$X_0 = Y_0 = 1,\ \frac{dX_\alpha}{d\alpha}\Big|_{\alpha=0} = \frac{dY_\alpha}{d\alpha}\Big|_{\alpha=0}; \tag{3.40}$$

that is, both curves originate at the identity (for $\alpha = 0$) and have a common tangent vector at it. From eq. (3.23), it follows that for a *one-parameter subgroup* $\{U_\alpha\}$, the tangent vector at the identity is its generator multiplied by $-i$.

Let $\{U_\alpha\}$ be the one-parameter subgroup of matrix group G. Substitute the parameter α for $\lambda\alpha$, where λ is a real number:

$$V_\alpha = U_{\lambda\alpha}. \tag{3.41}$$

Evidently, curve $\{V_\alpha\}$ is also a one-parameter subgroup,

$$V_{\alpha_1+\alpha_2} = U_{\lambda(\alpha_1+\alpha_2)} = U_{\lambda\alpha_1+\lambda\alpha_2} = U_{\lambda\alpha_1} \cdot U_{\lambda\alpha_2} = V_{\alpha_1} \cdot V_{\alpha_2}, \tag{3.42}$$

which is called a *product* of one-parameter subgroup $\{U_\alpha\}$ and the *real number* λ. The meaning of the definition is that the "speed" along one-parameter subgroup increases by λ times. The generator of the subgroup, in its turn, is multiplied by λ:

$$\frac{dV_\alpha}{d\alpha}\Big|_{\alpha=0} = \frac{dU_{\lambda\alpha}}{d\alpha}\Big|_{\alpha=0} = \lambda\frac{dU_\alpha}{d\alpha}\Big|_{\alpha=0}. \tag{3.43}$$

Let $\{U_\alpha\}$, $\{V_\alpha\}$ be two one-parameter subgroups of a matrix group G. Construct a matrix curve $\{W_\alpha\} = \{U_\alpha V_\alpha\}$. Since multiplication is generally not commutative, the curve is not generally a one-parameter subgroup. Since $W_0 = U_0 V_0 = 1$, the curve originates from the identity. Find its tangent vector at this point:

$$\frac{dW_\alpha}{d\alpha}\Big|_{\alpha=0} = \frac{dU_\alpha}{d\alpha}\Big|_{\alpha=0} \cdot V_0 + U_0\frac{dV_\alpha}{d\alpha}\Big|_{\alpha=0} = \frac{dU_\alpha}{d\alpha}\Big|_{\alpha=0} + \frac{dV_\alpha}{d\alpha}\Big|_{\alpha=0}. \tag{3.44}$$

Designate A and B as the generators of subgroups $\{U_\alpha\}$ and $\{V_\alpha\}$, respectively; then the tangent vector to $\{U_\alpha V_\alpha\}$ at the identity is $-i(A + B)$. Construct a one-parameter subgroup $\{W_\alpha\} = \{e^{-i\alpha C}\}$ with a tangent vector at the identity $C = -i(A + B)$; that is, the subgroup is tangent at the identity to the curve $\{U_\alpha V_\alpha\}$; this subgroup is called the *sum* of subgroups $\{U_\alpha\}$, $\{V_\alpha\}$.

The meaning of this definition is that such one-parameter subgroup most closely approximates $\{U_\alpha V_\alpha\}$ near identity: matrix $W_\alpha = e^{-i\alpha C}$ differs from the product $U_\alpha V_\alpha = e^{-i\alpha A} e^{-i\alpha B}$ for small α by the value of the second order with respect to α. It can be shown that such one-parameter subgroup is unique. Thus, for small α and first-order accuracy,

$$W_\alpha \approx U_\alpha V_\alpha \tag{3.45}$$

Therefore, the generator of the sum of one-parameter subgroups is the sum of their generators.

The same result is obtained if the product of subgroups is taken in the reverse order $\{V_\alpha U_\alpha\}$; that is, the sum does not depend on the order of the multiplied subgroups. We can prove that addition and multiplication by real numbers satisfy also all other requirements of a vector space. Thus, *one-parameter subgroups of a matrix Lie group constitute a real vector space*.

Note that we define no multiplication by *complex* numbers for one-parameter subgroups.[22] If a generator A of subgroup $\{U_\alpha\}$ is multiplied by i, the obtained matrix may be a generator of no one-parameter subgroup; but even if such a subgroup exists, it is not considered a product of $\{U_\alpha\}$ and i.

In the vector space of one-parameter subgroups, introduce another operation. Let $\{U_\alpha\}$, $\{V_\alpha\}$ be the one-parameter subgroups of a matrix group. Construct a curve $\{W_\alpha\}$:

$$W_\alpha = U_\alpha V_\alpha U_\alpha^{-1} V_\alpha^{-1}. \tag{3.46}$$

This expression "measures the noncommutativity" of the subgroups: the identity $\{W_\alpha\}$ is equivalent to $U_\alpha V_\alpha = V_\alpha U_\alpha$. Therefore, noncommutativity is measured by the deviation of W_α from the identity of the group. Substituting (eq. (3.22)) U_α^{-1}, V_α^{-1} for $U_{-\alpha}$, $V_{-\alpha}$ and differentiating, we find that tangent vector to $\{W_\alpha\}$ at the identity is zero, and therefore gives no information about the "measure of noncommutativity" for small α. Write our multipliers as Taylor's series

$$\begin{aligned} U_\alpha &= e^{-i\alpha A} = 1 - i\alpha A - \tfrac{\alpha^2}{2} A^2 + \cdots, \quad & V_\alpha &= e^{-i\alpha B} = 1 - i\alpha B - \tfrac{\alpha^2}{2} B^2 + \cdots, \\ U_\alpha^{-1} &= U_{-\alpha} = 1 + i\alpha A - \tfrac{\alpha^2}{2} A^2 + \cdots, \quad & V_\alpha^{-1} &= V_{-\alpha} = 1 + i\alpha B - \tfrac{\alpha^2}{2} B^2 + \cdots, \end{aligned} \tag{3.47}$$

22 In general, there is no reasonable way to define such operation.

and then multiply them, in compliance with the given order and accuracy up to α^2; so we have

$$W_\alpha = 1 - \alpha^2(AB - BA) + \cdots \tag{3.48}$$

This shows that $W_\alpha - 1$ is of the second order of smallness with respect to α. Let $\beta = \alpha^2$ and $Z_\beta = W_{\sqrt{\beta}} = 1 - \beta(AB - BA) + \cdots$. The tangent vector to this curve

$$\frac{dZ_\beta}{d\beta}|_{\beta=0} = -(AB - BA), \tag{3.49}$$

is, generally speaking, nonzero and can be used as a "measure" of noncommutativity. Construct a one-parameter subgroup $\{e^{-i\alpha C}\}$ tangent to the curve $\{Z_\alpha\}$ at the identity. To do this, take $C = \frac{1}{i}(AB - BA)$. This parameter subgroup is called a *commutator* of one-parameter subgroups $\{U_\alpha\}, \{V_\alpha\}$. Its generator is constructed from the generators A, B of one-parameter subgroups by usual commutation of matrices $[A,B] = AB - BA$ and dividing it by i.[23]

Consider, for example, a unitary group U_n. In this case, the generators of Lie algebra are Hermitian, operations of addition and multiplication by real numbers again produce Hermitian operators, that is, generators of $U(n)$. Multiplication by i gives not Hermitian matrices which are not generators of the group, and hence, the operation has no relation to operations defined on one-parameter subgroups. Further, if A, B are the Hermitian operators, then, denoting A^+ the adjoint operator with matrix ${}^tA^*$, obtain $A^+ = A$, $B^+ = B$,

$$\left(\frac{1}{i}[A, B]\right)^+ = -\frac{1}{i}(AB - BA)^+ = -\frac{1}{i}(B^+A^+ - A^+B^+) = \frac{1}{i}(AB - BA) = \frac{1}{i}[A, B], \tag{3.50}$$

so that the operation of commutation applied to generators again gives a Hermitian operator, that is, a generator of the group. Describe again the relationship between the operations with one-parameter subgroups of a matrix Lie group and operations with their generators by the following scheme:

$$\begin{array}{r|l} \{U_\alpha = e^{-i\alpha A}\} & A \\ \{V_\alpha = e^{-i\alpha B}\} & B \\ \text{Sum } \{U_\alpha\} \text{ and } \{V_\alpha\} & A + B \\ \text{Real multiple } \lambda\{U_\alpha\} & \lambda A \\ \text{Commutator } \{U_\alpha\} \text{ and } \{V_\alpha\} & \frac{1}{i}[A, B] \end{array} \tag{3.51}$$

23 This discrepancy does not arise in the mathematical literature, and one-parameter groups are written as $U_\alpha = e^{\alpha X}$, $V_\alpha = e^{\alpha Y}$, whence $Z_\alpha = 1 + \alpha[X,Y]$; the generators X,Y commute like the subgroups they generate. In Physics, this complication is done to ensure that generators in unitary representations are Hermitian operators.

Now consider *general* Lie groups which need not necessarily be matrix groups. In the general case, the elements of G can be only multiplied by each other, but, unlike matrices and operators, they cannot be added or multiplied by numbers.[24] The concept of one-parameter subgroup remains the same: it is a family of such elements $\{g_\alpha\}$ that

$$g_{\alpha_1+\alpha_2} = g_{\alpha_1} \cdot g_{\alpha_2}. \tag{3.52}$$

However, generators cannot be build for one-parameter subgroups, because in the general case, the procedure (3.23) is impossible, as ii implies nongroup operations. Nevertheless, the operations on one-parameter subgroups such as addition, multiplication by real numbers, and commutation defined above for matrices can readily be extended to the general case with the only difference that one-parameter subgroups cannot be defined by generating matrices and operations on one-parameter subgroups cannot be substituted by matrix operations on their generators as is described in the right side of scheme (3.51), because in the general case, the right side of the scheme does not exist.

Define a concept of a "curve" on a Lie group G. Curve is a family of elements of group $\{g_\alpha\}$ which depends on a real parameter α. A curve is called continuously differentiable if local coordinates $(\alpha_1, \ldots, \alpha_n)$ of element g_α are continuously differentiable functions of α in a vicinity of each value α_0:

$$\alpha_1 = \alpha_1(\alpha), \ldots, \alpha_n = \alpha_n(\alpha). \tag{3.53}$$

Compare this definition with a continuously differentiable curve $r = r(\alpha)$ defined by three scalar functions $x = x(\alpha)$, $y = y(\alpha)$, and $z = z(\alpha)$ in Euclidian space, or with a curve in the space of matrices $X(\alpha)$ defined by scalar functions x_{ij}. The change of local coordinates gives other continuously differentiable functions (eq. (3.53)) (e.g. $\beta_1(\alpha), \ldots, \beta_n(\alpha)$); therefore, the definition of a continuously differentiable curve does not depend on the choice of local coordinates. By analogy with tangent vector defined at $r(\alpha)$ by derivatives $\frac{dx(\alpha)}{d\alpha}, \frac{dy(\alpha)}{d\alpha}, \frac{dz(\alpha)}{d\alpha}$, or tangent vector to a matrix curve $X(\alpha)$ by derivatives $\frac{dx_{ij}(\alpha)}{d\alpha}$, we can define *components of the tangent vector* at a point of the curve $\{g_\alpha\}$ by the numbers in local coordinates $\frac{d\alpha_1(\alpha)}{d\alpha}, \ldots, \frac{d\alpha_n(\alpha)}{d\alpha}$, which transform under a change of coordinates as

$$\frac{d\beta_i}{d\alpha} = \sum_{j=1}^{n} \frac{\beta_i}{\partial\alpha_j} \frac{d\alpha_j}{d\alpha}. \tag{3.54}$$

There is no intuitive interpretation of the "tangent vector," but we will assume that numbers $\frac{d\alpha_j(\alpha)}{d\alpha}, \frac{d\beta_i(\alpha)}{d\alpha}, \ldots$, which transform according to eq. (3.54), define a *tangent vector*

24 Note that also in the case of groups consisting of matrices and operators, when addition of elements and their multiplication by numbers make sense, these operations are not group operations, that is, generally speaking, take out of the group.

at point g_α. Now we can define the notion of *tangency* of curves. Curves $\{g_\alpha\}$ *and* $\{h_\alpha\}$ are said to be tangent at point $g_\alpha = h_\alpha$ if they have a common tangent vector at this point. In other words, if the curves have coordinates $\{\alpha_i^{(g)}(\alpha)\}$ *and* $\{\alpha_i^{(h)}(\alpha)\}$, respectively, then

$$\frac{d\alpha_i^{(g)}(\alpha)}{d\alpha} = \frac{d\alpha_i^{(h)}(\alpha)}{d\alpha} \quad (i = 1, \ldots, n). \tag{3.55}$$

As is seen from eq. (3.54), this definition does not depend on the choice of local coordinates. Designate $\frac{dg_\alpha}{d\alpha}$ the tangent vector to curve $\{g_\alpha\}$.

It can be proved that each parameter subgroup $\{g_\alpha\}$ of a Lie group G is a continuously differentiable curve. In the case of a matrix group, tangent vectors to one-parameter subgroups at the identity of the group can be shown to be in a one-to-one correspondence with their generators:

$$\frac{dg_\alpha}{d\alpha}\Big|_{\alpha=0} = -iA. \tag{3.56}$$

In general, tangent vectors have no visual representation in the form of a matrix.

With the concept of tangent curves, we can apply three above operations on one-parameter subgroups to general Lie groups. The operation of *multiplying of a one-parameter subgroup* $\{g_\alpha\}$ *of group G by a real number* is defined exactly the same way as above:

$$\lambda\{g_\alpha\} = \{g_{\lambda\alpha}\} \tag{3.57}$$

For tangent vectors at the identity, it means that

$$\frac{dg_{\lambda\alpha}}{d\alpha}\Big|_{\alpha=0} = \lambda\frac{dg_\alpha}{d\alpha}\Big|_{\alpha=0}, \tag{3.58}$$

which has the following intuitive meaning: for small α, the element $g_{\lambda\alpha}$ is "λ times farther" from the identity than element g_α, that is, the motion along the subgroup is λ times faster when multiplied by λ.

The sum of two one-parameter subgroups $\{g_\alpha\}, \{h_\alpha\}$ of group G is defined as a one-parameter subgroup $\{f_\alpha\}$tangent to the curve $\{g_\alpha h_\alpha\}$at the identity:

$$\frac{df_\alpha}{d\alpha}\Big|_{\alpha=0} = \frac{d}{d\alpha}(g_\alpha h_\alpha)\Big|_{\alpha=0}. \tag{3.59}$$

Intuitively, this definition means that for small α elements, f_α and $g_\alpha h_\alpha$ coincide up to small quantities of high order with respect to α. It can be verified that eq. (3.59) uniquely defines a one-parameter subgroup $\{f_\alpha\}$.

Commutator of two one-parameter subgroups $\{g_\alpha\}, \{h_\alpha\}$ of group G is defined as a one-parameter subgroup $\{f_\alpha\}$ tangent at the identity to the curve $\{g_{\sqrt{\alpha}}h_{\sqrt{\alpha}}g_{\sqrt{\alpha}}^{-1}h_{\sqrt{\alpha}}^{-1}\}$ $(\alpha \geq 0)$:

$$\frac{df_\alpha}{d\alpha}\Big|_{\alpha=0} = \frac{d}{d\alpha}\left(g_{\sqrt{\alpha}}h_{\sqrt{\alpha}}g_{\sqrt{\alpha}}^{-1}h_{\sqrt{\alpha}}^{-1}\right)\Big|_{\alpha=0}. \tag{3.60}$$

The reason of introducing this definition is the same as for matrices: a tangent vector $\frac{df_\alpha}{d\alpha}\big|_{\alpha=0}$ "measures" the noncommutativity of subgroups $\{g_\alpha\}$, $\{h_\alpha\}$ (see eqs. (3.46)–(3.49)). It can be proved that eq. (3.59) uniquely defines the one-parameter subgroup $\{f_\alpha\}$.

A set of one-parameter subgroups of Lie group G with operations of addition, multiplication by real numbers, and commutation is called *Lie algebra* of group G. Designate it g.

In general, *algebra* is **a** set a with operations of addition of elements $a + b$, multiplication of elements ab, and multiplication of elements by (real or complex) numbers λ, which satisfies the following conditions:

(1) **a** is an Abelian group with respect to addition;
(2) multiplication of elements is distributive:

$$a(b + c) = ab + ac,\ (b + c)a = ba + ca; \tag{3.61}$$

(3) multiplication by numbers is distributive: $\lambda(a + b) = \lambda a + \lambda b$, $(\lambda + \mu)a = \lambda a + \mu a$;
(4) $\lambda(\mu a) = (\lambda\mu)a$;
(5) $(\lambda a)b = a(\lambda b) = \lambda(ab)$;
(6) $1{\cdot}a = a$ (where 1 is the unity).

Multiplication of elements is not assumed commutative or associative. The algebra of matrices is associative but not commutative. As we will see, Lie algebras are neither commutative nor associative. In modern mathematics, algebras are generalizations of real and complex numbers.

For Lie algebras, commutation operation is used instead of multiplication, and *real* numbers are taken as numerical factors. Let small Latin letters a,b,c,... denote one-parameter subgroups. Then $a + b$ denotes the addition operation, λa denotes the multiplication, and $[a,b]$ denotes the commutation.[25] The operations in Lie algebras satisfy conditions (3.12)–(3.17); for example, the distributivity of multiplication means, applied to the commutation operation, that the following identities are true:

$$[a + b, c] = [a, c] + [b, c],\ [c, a + b] = [c, a] + [c, b], \tag{3.62}$$

and the condition (3.16) has the form

$$[\lambda a, b] = [a, \lambda b] = \lambda[a, b]. \tag{3.63}$$

However, Lie algebras have another special property which distinguishes them as a special class of algebras. Namely, they satisfy the identity

$$[a, b] = -[b, a], \tag{3.64}$$

25 For matrix Lie groups, when the elements of Lie algebras (one-parameter subgroups $a,b,\ldots$) can be replaced by their generating generators $A,B,\ldots$, commutator $[a,b]$ corresponds to the generator $\frac{1}{i}[A, B] = \frac{1}{i}(AB - BA)$.

which replaces the condition of commutativity of the product; this property of Lie algebras is called *anticommutativity*. Further, there is another identity which connects together three elements of Lie algebras; it replaces the associativity of the product and is called the *Jacobi identity*:

$$[a,[b,c]]+[b,[c,a]]+[c,[a,b]]=0. \tag{3.65}$$

Identity (3.65) is easy to remember because its second and third terms are obtained from the first by cyclic permutation of the multipliers. An obvious consequence of eq. (3.64) for $a = b$ is the identity,

$$[a,a]=0. \tag{3.66}$$

We do not prove here the properties (3.61), (3.64), and (3.65) of Lie algebras in the general case; but in the case of matrix groups, operations over one-parameter subgroups can be replaced by operations over their generators, the proof is not difficult. For example, anticommutativity is proved as

$$[A,B]=AB-BA=-(BA-AB)=-[B,A], \tag{3.67}$$

and the Jacobi identity as

$$\begin{aligned}[A[B,C]]&=A[B,C]-[B,C]A=A(BC-CB)-(BC-CB)A\\&=ABC-ACB-BCA+CBA\end{aligned} \tag{3.68}$$

and two other similar expressions.

For some matrix groups, we already can find their Lie algebra. If one-parameter subgroups of a matrix group can be defined by their generators, we will say (when it creates no confusion) that these generators *constitute* a Lie algebra. As we saw, generators of group $U(n)$ are Hermitian matrices, and every Hermitian matrix A generates a one-parameter subgroup of unitary matrices by eq. (3.31). So, *Lie algebra of* $U(n)$ *consists of all Hermitian matrices*. We have already verified by direct calculations (eq. (3.50)) that a commutator of Hermitian matrices divided by i is also a Hermitian matrix. Group SU(n) is a subgroup of $U(n)$, so all its generators are Hermitian. But now there is an additional requirement, $\det|U| = 1$, and from eq. (3.10) obtain $e^{tr(-i\alpha A)} = 1$, whence $tr\, A = 0$. Thus, *Lie algebra of* SU(n) *consists of traceless Hermitian matrices*. It is easily verified that a commutator of traceless matrix (in fact, any matrix) is a traceless matrix:

$$tr[A,B]=tr(AB-BA)=tr(AB)-tr(BA)=0, \tag{3.69}$$

as the trace of the product of matrices does not depend on their order. Orthogonal group $O(n)$ is a subgroup of $U(n)$ consisting of matrices with real elements; therefore, *its Lie algebra consists of Hermitian matrices*, and, as follows from eq. (3.31), with *purely imaginary elements*. Group SO(n) differs from $O(n)$ by the an additional

requirement $\det|U| = 1$, that is, matrices of its Lie algebra must have a zero trace; but for purely imaginary Hermitian matrices, this requirement is always satisfied, so the Lie algebra for SO(n) is the same as for $O(n)$. This is also seen from the fact that one-parameter subgroups of the group of orthogonal matrices $\{O_\alpha\}$ originate from the identity, and since $\det|O_\alpha| = \pm 1$ obtain from the continuity that $\det|O_\alpha| = 1$ for all α; it means that one-parameter subgroups $O(n)$ and SO(n) coincide. As is easily verified, *Lie algebra of the general linear group* GL(n,C) *consists of matrices of order n* (with complex elements); *Lie algebra of the unimodular group* SL(n,C) (matrices with determinant 1) *consists of all traceless matrices*.

In the case of matrix groups, there is a general formula relating a Lie group and its Lie algebra (defined by its generators). Let A be the generator of group G, and $\{e^{-i\alpha A}\}$ is its corresponding one-parameter subgroup. Then $U_\alpha = e^{-i\alpha A}$ for all α belongs to G; in particular, for $\alpha = 1$, we find that matrix

$$U_\alpha = e^{-iA} \tag{3.70}$$

belongs to G. Comparison of eq. (3.70) with the formula of exponential map eq. ((3.6)) gives $X = -iA$ and that sufficiently small matrices A of Lie algebra $\mathfrak{g}$ are in a continuous one-to-one correspondence (eq. (3.70)) with those matrices U of group G which are sufficiently close to the identity. We have used this in Section 3.1 to calculate the dimensions of some Lie groups. The Lie algebra of a matrix group is a real vector space which is, as can be shown, finite.

Replace the elements of the corresponding Lie algebra $\mathfrak{g}$, that is, one-parameter subgroups of G, by their generators. Then a basis $A_1, \ldots, A_n$ can be chosen in $\mathfrak{g}$ such that all operators of $\mathfrak{g}$ are linear combinations with real coefficients:

$$A = \alpha_1 A_1 + \cdots + \alpha_n A_n. \tag{3.71}$$

Since for sufficiently small α_i operators, A belong to the vicinity related by the exponential correspondence to the identity of G, we can take coefficients $\alpha_1, \ldots, \alpha_n$ as local coordinates in the vicinity of the identity of this group. Thus, *the dimension of a Lie algebra coincides with the dimension of its Lie group*. From eqs. (3.70) and (3.71) obtain the representation for the elements of matrix group sufficiently close to the identity:

$$U = e^{-i\sum_{k=1}^{n} \alpha_k A_k}. \tag{3.72}$$

Construct, for example, a basis of the Lie algebra of SO(3). Matrices of this Lie algebra – i.e. Hermitian matrices with purely imaginary elements – are expressed as a linear combination with real coefficients of three matrices A_i (eq. (3.36)) which generate the subgroups of rotations about coordinate axes:

$$A = \alpha_1 A_1 + \alpha_2 A_2 + \alpha_3 A_3. \tag{3.73}$$

If $B = \beta_1 A_1 + \beta_2 A_2 + \beta_3 A_3$ is another matrix of Lie algebra, then

$$[A, B] = \left[\sum_{i=1}^{3} \alpha_i A_i, \sum_{j=1}^{3} \beta_j A_j\right] = \sum_{i,j=1}^{3} \alpha_i \beta_j [A_i, A_j], \tag{3.74}$$

and all commutators of this algebra are found from the commutators of basic matrices A_i:

$$[A_1, A_2] = iA_3, \quad [A_2, A_3] = iA_1, \quad [A_3, A_1] = iA_2. \tag{3.75}$$

Similarly, matrices τ_i (eq. (3.37)) form a basis of the Lie algebra of group SU(2) with commutators

$$[\tau_1, \tau_2] = i\tau_3, \quad [\tau_2, \tau_3] = i\tau_1, \quad [\tau_3, \tau_1] = i\tau_2 \tag{3.76}$$

For GL(n,C) group, the basis of its Lie algebra (consisting of all matrices) are matrices B^i_j with a nonzero element at the intersection of the j-th row and the i-th column, and matrices iB^i_j $(i, j = 1, \ldots, n)$. Their commutators are

$$\begin{aligned} &[B^i_j, B^k_l] = \delta^i_l B^k_j - \delta^k_j B^i_l, \ [iB^i_j, iB^k_l] = -\delta^i_l B^k_j + \delta^k_j B^i_l, \\ &[iB^i_j, B^k_l] = [B^i_j, iB^k_l] = i\delta^i_l B^k_j - i\delta^k_j B^i_l. \end{aligned} \tag{3.77}$$

where $\delta^i_l = 0$ for $i \neq l$ and $\delta^i_j = 1$. The reader is advised to verify that matrices $A^i_j = B^i_j - \frac{1}{n}(tr\, A^i_j) \cdot 1$ are related by equation $\sum_{i=1}^{n} A^i_i = 0$ and that $n^2 - 1$ independent matrices A^i_j and corresponding matrices iA^i_j form the basis of the Lie algebra of SL(n,C), and to find commutation relations for the matrices of this basis.

It can be proved that for any (not necessarily matrix) Lie group, its Lie algebra is finite and has the same dimension as its Lie group. If we choose a basis $a_i (i = 1, \ldots, n)$ in the Lie algebra, then any element a of the algebra is represented as

$$a = \sum_{i=1}^{n} \alpha_i a_i \tag{3.78}$$

and the commutator of any a, b has the form

$$[a, b] = \left[\sum_{i=1}^{n} \alpha_i a_i, \sum_{j=1}^{n} \beta_j a_j\right] = \sum_{i,j=1}^{n} \alpha_i \beta_j [a_i, a_j] \tag{3.79}$$

so that the commutation operation in Lie algebra is completely determined by the commutators of its basic elements $[a_i, a_j]$. Expressing these commutators in terms of the basis, obtain *commutation relations* for the Lie algebra:

$$[a_i, a_j] = \sum_{k=1}^{n} c^k_{ij} a_k \tag{3.80}$$

Real numbers c^k_{ij} are called *structural constants* of the Lie algebra. These constants, according to eq. (3.79), completely determine the commutation operation, and thereby the structure of the Lie algebra. Structural constants depend on the selected basis $\{a_i\}$; the basis is usually chosen the way that commutation relations be as easy

as possible. If the basis changes, the structure constants transform by the tensor law, which is reflected in their designations.

If G is a matrix group, then the commutation operation for *generators* has the form $\frac{1}{i}[A, B]$ (eq. (3.51)); equation (3.78) becomes

$$A = \sum_{k=1}^{n} \alpha_i A_i, \tag{3.81}$$

with real α_i, and commutation relations (eq. (3.80)) take the form

$$[A_i, A_j] = i \sum_{k=1}^{n} c_{ij}^k A_k \tag{3.82}$$

with the same structural constants as in eq. (3.79). Equations (3.75) and (3.76) are examples of such relations; relations (3.76) can be written in the same form if i on the right side is factored out.

Since Lie algebras have *linear* structure of a real vector space with linear operation of commutation, transition from Lie group to its Lie algebra has important advantages. This operation obeys eq. (3.67) to replace the commutativity operation. Situation is more complicated for a *group*, where there is no linear structure and, generally speaking, multiplication is not commutative. The role of commutation can be explained as follows. The structure of the Lie algebra is completely determined by a finite set of numbers or structural constants. It turns out that we can reduce group operations in Lie groups (in any case, in the vicinity of the identity) to the operations in its Lie algebra, addition, multiplication by real numbers, and commutation, so the structure of the Lie algebra determines, at least locally, the structure of its Lie group (Campbell–Hausdorff formula). Reducing the study of Lie groups to their Lie algebras, we can then use the methods of linear algebra. As we will see, Lie algebras are also useful to construct representations of Lie groups.

There is a convenient way to study matrix Lie groups with the help of generators which reduce operations on one-parameter subgroups to the operations on matrices. This, in particular, made it possible to find a general form of generators and commutation relations for some matrix groups, that is, fully clarify the structure of their Lie algebras. For nonmatrix Lie groups, there is no such an effective method yet. Meanwhile, some important Lie groups used in physics are not matrix groups: for example, all groups containing translations, such as the isometry group, Galilean group, and Poincare group. As we will see, *faithful representations* provide a tool necessary to study nonmatrix groups.

3.3 Representations of Lie groups

Let G denote the Lie group and R denote the finite or infinite complex vector space. Let each element g of group G correspond to a linear operator T_g which acts in R and the following conditions are fulfilled,

(1) $T_{g_1 g_2} = T_{g_1} T_{g_2}$ for any g_1, g_2 from G; (3.83)

(2) $T_e = 1$, where e is the identity of G, and 1 is the identity operator.

The correspondence between operators T_g and elements g is called a *representation* of G in the space R. If $g_1 g_2 = e$, then from eqs. (3.83) and (3.84), obtain $T_{g_1} T_{g_2} = 1$, whence

$$T_{g^{-1}} = (T_g)^{-1} \tag{3.84}$$

If different elements g correspond to different operators T_g, the representation $\{T_g\}$ is called *faithful*. In this case, there is a one-to-one mapping between the elements of the group and the operators to represent them, so that the mapping preserves group operations, that is, group G is *isomorphic* to the group of operators $\{T_g\}$. Isomorphic groups differ only as far as the specific form of their elements rather than algebraic relations between them. Yet in some cases, for example, when the elements of the original group have direct physical meaning, it is not useful to use the isomorphic group. This is the case, for example, of the isometry group or Poincare group. Therefore, we will always distinguish between the original group and its isomorphic models (e.g. exact representations).

Matrix Lie groups, by definition, have a faithful representation in the space with the dimension equal to the order of the matrices (see eq. (3.19)). Each matrix is represented by a linear operator depending on the chosen basis. In fact, in Section 3.2, we used basis vectors $e_1 = (1, 0, \ldots, 0)$, $e_2 = (0, 1, \ldots, 0)$, $\ldots$, $e_n = (0, 0, \ldots, 1)$ and vector $z = (z_1, \ldots, z_n)$ was decomposed as $z = \sum_{k=1}^{n} z_k e_k$. This representation of matrix groups has no special mathematical term, but it is often called "fundamental" in physical literature.

Let G be the Lie group and $\{T_g\}$ its representation in C^n. In any basis $(e_1, \ldots, e_n)$ operators T_g are defined by matrices $U = (u_{ij})$ which act on vectors $z = \sum z_k e_k$ according to eq. (3.19), and the coordinates of vectors z and $z' = Uz$ are taken in the same basis (e_i). Consider another basis (f_l),

$$e_k = \sum_{l=1}^{n} \varphi_{lk} f_l \quad (k = 1, \ldots, n). \tag{3.85}$$

Let w_i denote the coordinates of z in the new basis, then

$$\sum_{k=1}^{n} z_k e_k = \sum_{i,k=1}^{n} z_k \varphi_{ik} f_i = \sum_{i=1}^{n} \left(\sum_{k=1}^{n} \varphi_{ik} z_k \right) f_i = \sum_{i=1}^{n} w_i f_i \tag{3.86}$$

whence

$$w_i = \sum_{k=1}^{n} \varphi_{ik} z_k \tag{3.87}$$

The coordinates of the transformed vector z' are expressed in the new basis as

$$w'_i = \sum_{k=1}^{n} \varphi_{ik} z'_k = \sum_{k,l=1}^{n} \varphi_{ik} u_{kl} z_l = \sum_{k,l,j=1}^{n} (\varphi_{ik} u_{kl} \varphi_{lj}^{-1}) w_j \tag{3.88}$$

This means that operator T_g in the new basis is represented by matrix

$$U' = \Phi U \Phi^{-1} \tag{3.89}$$

Equation (3.89) gives the relation between the matrices of the *same* representation in different bases of space R. Similarly looks the relationship between *equivalent* representations discussed in Section 1.3. Denote $\{T_g\}$ and $\{T'_g\}$ the representations of the same group G in spaces R and R′, respectively. Let Φ be the *isomorphism* between these spaces, that is, it is a linear operator defining a one-to-one mapping between R and R′ such that for $z' = T_g z$ and $w = \Phi z$, $w = \Phi z'$, the equation $T'_g w = w'$ is true. In this case, the representations $\{T_g\}$, $\{T'_g\}$ are called *equivalent*. Evidently, equivalent representations have similar structure: each vector z from R is replaced by its "copy" $w = \Phi z$ from R′, and representation $\{T'_g\}$ works with the "copies" the same way as $\{T_g\}$ works with their "originals." The equivalence of operators is expressed by the equation

$$T'_g \Phi = \Phi T_g, \quad \text{or} \quad T'_g = \Phi T_g \Phi^{-1} \quad \text{for all } g. \tag{3.90}$$

As a special case, both representations can be also defined in the same space R. Isomorphic mapping of space R on itself is called an *automorphism* of R. If R is finite and all its operators (including the automorphism) are written in the same basis, eq. (3.90) can be replaced by a matrix equation of the same form as eq. (3.89).

Let R denotes the Hilbert space. If all operators of representation T_g are unitary, that is,

$$\langle T_g v | T_g w \rangle = \langle v | w \rangle, \tag{3.91}$$

for all vectors v,w, the representation $\{T_g\}$ is called *unitary*. If group G is compact, then for any of its finite-dimensional representation $\{T_g\}$, a positive definite scalar product can be defined in the space of representations such that $\{T_g\}$ becomes unitary. Having in mind physical applications, we will further consider only unitary representations for both compact and noncompact groups.

From now on, we consider only Hilbert representation spaces. In Hilbert spaces, similar to the Euclidean space, a *norm* of vectors is defined using scalar product:

$$\|v\| = \sqrt{\langle v | v \rangle} \tag{3.92}$$

With respect to this norm, a concept of *convergence* of vectors can be defined: $v_n \to v_0$ for $n \to \infty$, if $\|v_n - v_0\| \to 0$. Hilbert space is *complete* if its sequences obey a property similar to "Cauchy's test" for numeric sequences: any sequence of vectors $\{v_n\}$ such that $\|v_m - v_n\| \to 0$ for $m, n \to \infty$ converges. It can be verified that Hilbert space of

functions $\psi(x, y, z)$ with square-integrable module is complete. We will assume that all Hilbert spaces are complete. Further we will consider *subspaces* of Hilbert spaces. A Hilbert space R' is called a subspace of a Hilbert space R, if all vectors of R' belong to R (i.e. R' is a subset of R), and if the scalar product in R' is the same as in R.[26]

Let R' denotes the subspace of R and representation $\{T_g\}$ of group G is defined in R. If all operators of representation $\{T_g\}$ carry the vectors of R' into the vectors of R', then R' is called an *invariant subspace* of representation $\{T_g\}$. In this case, the representation $\{T_g\}$ defines a representation of the same group G in the subspace R': it is obtained by applying operators $\{T_g\}$ to vectors R' only. Such representation is said to be *induced* by the given representation $\{T_g\}$. If space R contains no invariant subspaces of $\{T_g\}$ other than the whole R and zero subspace (consisting only of the zero vector), representation $\{T_g\}$ is called *irreducible*.

Suppose that Hilbert space R contains mutually orthogonal subspaces R_k (i.e. for any vector v_k from R_k and v_l from $\mathsf{R}_l (k \neq l)$ the scalar product $\langle v_k | v_l \rangle = 0$). Space R is decomposed into *orthogonal sum* of subspaces R_k, if each vector v of space R is uniquely represented in the form

$$v = v_1 + v_2 + \cdots , \tag{3.93}$$

where v_k belongs to R_k. (In the case of an infinite number of subspaces, the sum in eq. (3.93) is understood as the sum of a convergent series, that is, $\|v - (v_1 + \ldots + v_n)\| \to 0$ for $n \to \infty$.)

Decomposition into an orthogonal sum can be written as

$$\mathsf{R} = \mathsf{R}_1 \oplus \mathsf{R}_2 \oplus \cdots \tag{3.94}$$

A wide class of Lie groups, including all those which we need, the following theorem is true: representation space of a group can be decomposed into orthogonal sum of invariant subspaces irreducible with respect to this representation. In Chapter 1, we decomposed an infinite-dimensional representation of the rotation group into irreducible representations (see eqs. (1.33) and (1.34)). For finite-dimensional representations, an orthonormal basis $\{e_j\}$ can be chosen in R such that all its vectors belong to subspaces R_k. Then, if e_j belongs to R_k, then all vectors $T_g e_j$ also belong to R_k and are therefore decomposed only by the basis vectors of R_k. If first basis vectors of R_1 are written down, then basis vectors R_2, and so on, then all matrices T_g take a "box form," and the dimensions of diagonal boxes are the same as the dimensions of R_1, R_2, …; matrices in these boxes represent irreducible representations in the corresponding subspaces.

26 It can be shown that subspaces as defined above are *closed*: if a sequence $\{v_n\}$ of vectors from R' converges in R to some vector v_0, then v_0 belongs to R'. In this book, we consider only closed subspaces.

Let G_1 denotes the subgroup of a Lie group G, and let it also be a Lie group (we will consider only such subgroups); suppose that $\{T_g\}$ is an irreducible representation of G in R. If only those operators of representation $\{T_g\}$ considered that g belongs to G_1, then a representation of the subgroup G_1 in the same space R is obtained. The described process is called a *reduction* of representation $\{T_g\}$ to the subgroup G_1. Reduced representation of subgroup G_1 is usually reducible and is decomposed into irreducible subspaces of the form (3.94). Reducing representations is important in physical applications. As was shown in Chapter 1, the space of Schrodinger ψ functions can be regarded as an irreducible space of some representation of the conformal group SO(4,2); the reduction of this representation to the subgroup SO(4) leads to the decomposition into irreducible representations SO(4) (eq. (1.33)), and further reduction to the subgroup SO(3) to the decomposition (eq. (1.34)).

Let G be a Lie group, g its Lie algebra, and $\{T_g\}$ representation of G in the space R. Each element g (i.e. each one-parameter subgroup $a = \{g_\alpha\}$ of group G) corresponds to the family of operators $\{T_{g_\alpha}\}$ and is easily seen that this family is a one-parameter subgroup of operators:

$$T_{g_{\alpha_1+\alpha_2}} = T_{g_{\alpha_1} g_{\alpha_2}} = T_{g_{\alpha_1}} T_{g_{\alpha_2}}, \tag{3.95}$$

and

$$T_{g_0} = T_e - 1 \tag{3.96}$$

where 1 means the identity operator regardless of the space. In Section 2.1, some examples of such operator subgroups were considered (see eqs. (2.13) and (2.14)). In contrast to the elements of the original one-parameter subgroup $\{g_\alpha\}$ (which generally allow only multiplication by each other), the elements of the representing one-parameter subgroup $\{T_{g_\alpha}\}$ can, similar to all operators, can also be added and multiplied by any complex number (since they act in a *complex* space R). This makes it possible to build a *generator* for $\{T_{g_\alpha}\}$ like it was done in eq. (3.23) for one-parameter subgroups of matrix groups:[27]

$$T_a = i \lim_{\alpha \to 0} \frac{T_{g_\alpha} - 1}{\alpha} = i \frac{dT_{g_\alpha}}{d\alpha}\Big|_{\alpha=0}. \tag{3.97}$$

This way a mapping $a \to T_a$ is defined: each element of Lie algebra g is associated with an operator acting in a representation of Lie group G. It can be proved that for this

27 For infinite-dimensional representations, operators T_a may not be defined on all vectors of the representation space. We can always select a subset L where all operators T_a are defined such that L is *linear*, that is, together with any two vectors contains their sum, and together with each vector contains its multiple; L is everywhere *dense*, that is, for each vector of the representation space, there is an arbitrarily close vector of L. In the case of a function space, L can be composed of continuously differentiable functions.

correspondence, the operations in the Lie algebra g (i.e. operations on one-parameter subgroup G described in Section 3.2) transform into similar operations with the operators to represent them:

(1) If $c = a + b$, then $T_c = T_a + T_b$;

(2) If $c = \lambda a$, where λ is a real number, then $T_c = \lambda T_a$; (3.98)

(3) If $c = [a, b]$, then $T_c = \frac{1}{i}[T_a, T_b] = \frac{1}{i}(T_a T_b - T_b T_a)$.[28]

Mapping $a \to T_a$ is called a *representation* of the Lie algebra g *generated by the given representation of Lie group G*. The term can be used also in the case when there is no representation G; namely, if the elements a of algebra g are put in correspondence to operators T_a to act in space R, and the conditions (eq. (3.98)) are fulfilled, then we say that representation of g is defined in R.

A representation of Lie algebra g can be used to construct a representation (at least local, i.e., in a vicinity of the identity) of Lie group G generating Lie algebra g. It can be verified that there exists a vicinity ε of the identity of group G completely covered by one-parameter subgroups, and that the following conditions of "correct covering" are fulfilled: each one-parameter subgroup $\{g_\alpha\}$ has an initial curve corresponding to the parameter change $0 \le \alpha \le \alpha_0$ and lying entirely in ε. When parameter α is replaced by $\lambda\alpha(\lambda > 0)$, the initial curve $\{h_\alpha\}$, $0 \le \alpha \le \frac{1}{\lambda}\alpha_0$ is obtained, where $h_\alpha = \lambda_0$. These two initial curves are called *overlapping*. Then we have (1) each initial curve does not cross itself; (2) two initial curves either intersect only at the identity or overlap; (3) the whole vicinity ε is covered by the initial curves of one-parameter subgroups. Furthermore, we will take on each one-parameter subgroup its initial curve. Then each element belonging to ε, except the identity, belongs to some initial curve, and if it belongs to more than one curve, the curves overlap. Thus, with an accuracy up to overlapping, the initial curve of one one-parameter subgroup passes through each element $g \neq e$ of the vicinity ε. As we will see, this fact makes it possible to build a *one-to-one* (local) representation of group G in the vicinity ε. Suppose that subgroup $a = \{g_\alpha\}$ corresponds to operator T_a in the representation of its Lie algebra. Construct now a one-parameter subgroup of operators

$$T_a(\alpha) = e^{-i\alpha T_a} \tag{3.99}$$

similar to matrix group (eq. (3.31)). Associate the identity e of group a with the identity operator 1, and element $g_\alpha \neq e$ of a one-parameter subgroup a with operator $T_a(\alpha)$ with the same value of parameter α. If we take $\lambda\alpha = \{h_\alpha\}(\lambda = 0)$ instead of a, then by the definition of multiplication in Lie algebras, $h_\alpha = g_{\lambda\alpha}$, so that $g_\alpha = h_{\frac{1}{\lambda}\alpha}$. From eq. (3.98) it follows that $T_{\lambda a} = \lambda T_a$. If g_α belongs to a one-parameter subgroup λα (with the parameter $\frac{1}{\lambda}\alpha$), the corresponding operator, as follows from eq. (3.99), is

28 The factor $\frac{1}{i}$ is the result of transition from one-parameter subgroups to their generators, see eq. (3.51).

$$T_{\lambda a}\left(\frac{\alpha}{\lambda}\right) = e^{-i\frac{\alpha}{\lambda}T_{\lambda a}} = e^{-i\frac{\alpha}{\lambda}\lambda T_a} = e^{-i\alpha T_a} = T_a(\alpha). \tag{3.100}$$

This shows that the operator corresponding to g_α is independent of the change of the parameter in the one-parameter subgroup. Let $g_\alpha = g$, $T_a(\alpha) = T_g$. From eq. (3.98), it can be shown that $T_{g_1 g_2} = T_{g_1} T_{g_2}$, that is, correspondence $g \to T_g$ is a representation of G. This representation of the group generates the initial representation of the Lie algebra; indeed, in the representation $\{T_g\}$ the one-parameter subgroup $a = \{g_\alpha\}$ corresponds to the one-parameter subgroup $\{T_{g_\alpha} = T_a(\alpha)\}$ of the form (3.99) with generator T_a. If all operators T_a are Hermitian, then the resulting representation $\{T_g\}$ is unitary. In fact, the operator T_g is unitary if $\langle T_g v | T_g w\rangle = \langle v|w\rangle$ or (which is the same) $\langle T_g^+ T_g v|w\rangle = \langle v|w\rangle$ for all vectors v, w; in other words, the unitarity condition has the form

$$T_g^+ = T_g^{-1} \tag{3.101}$$

If $T_a^+ = T_a$, then eq. (3.101) is true:

$$T_g^+ = (e^{-i\alpha T_a})^+ = e^{i\alpha T_a^+} = e^{i\alpha T_a} = (e^{-i\alpha T_a})^{-1} = T_g^{-1}. \tag{3.102}$$

Consider, for example, the representation of the isometry group $M(3)$ in the space of ψ functions (3.25). One-parameter subgroup of translations $g_\alpha(x, y, z) = (x + \alpha, y, z)$ (eq. (3.30)) corresponds in this representation to a one-parameter subgroup of operators $T_{g_\alpha}\psi(x, y, z) = \psi(x - \alpha, y, z)$ (eq. (2.11)) with generator $\frac{1}{i}\frac{\partial}{\partial x}$ (eq. (2.12)). If we started with the representation of the Lie algebra, we would put operator $T_a = \frac{1}{i}\frac{\partial}{\partial x}$ into correspondence with the element $a = \{g_\alpha\}$. It is easily verified that this operator is Hermitian. Since wave functions vanish at infinity,[29] we have

$$\begin{aligned}\langle T_a^+\varphi|\psi\rangle = \langle\varphi|T_a\psi\rangle = \langle\varphi|\tfrac{1}{i}\tfrac{\partial\psi}{\partial x}\rangle = -i\int\varphi^*\frac{\partial\psi}{\partial x}d^3x = -i[\varphi^*\psi]_{x=-\infty}^{x=+\infty} + i\int\frac{\partial\varphi^*}{\partial x}\psi d^3x \\ = \int\left(\frac{1}{i}\frac{\partial\varphi}{\partial x}\right)^*\psi d^3x = \langle T_a\varphi|\psi\rangle\end{aligned} \tag{3.103}$$

A one-parameter subgroup of operators generated by T_a is constructed according to eq. (3.99):

$$T_a(\alpha) = e^{-i\alpha T_a} = e^{-\alpha\frac{\partial}{\partial x}} = 1 - \alpha\frac{\partial}{\partial x} + \frac{\alpha^2}{2!}\frac{\partial^2}{\partial x^2} - \frac{\alpha^3}{3!}\frac{\partial^3}{\partial x^3} + \cdots \tag{3.104}$$

The meaning of operator $T_a(\alpha)$ becomes clear when it is applied to function ψ. From Taylor's formula, obtain

29 For the most common wave functions, satisfying only the condition (1.1), this proof needs to be generalized, but the result remains the same. The same is true for the conclusion (eq. (3.105)) where Taylor expansion is not needed.

$$T_a(\alpha)\psi(x,y,z) = \psi(x,y,z) - \alpha\frac{\partial}{\partial x}\psi(x,y,z) + \frac{\alpha^2}{2!}\frac{\partial^2}{\partial x^2}\psi(x,y,z) - \frac{\alpha^3}{3!}\frac{\partial^3}{\partial x^3}\psi(x,y,z) + \cdots$$
$$= \psi(x-\alpha,y,z) \tag{3.105}$$

Thus, translation by α along axis x corresponds to the operator (eq. (2.11)), and again the representation of translations described in Section 2.1 is obtained. The reader is encouraged to verify similar calculations for rotations using rotation angle α about z axis and taking into account that $\frac{\partial}{\partial\alpha} = x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}$.

Lie algebra g is defined by its basis $\{a_k\}$ and commutation relations (eq. (3.80)). To construct a representation g in space R, it is enough to set a correspondence between the elements a_k of the basis and Hermitian operators T_{a_k} acting in this space and satisfying the following commutation relations:

$$[T_{a_i}, T_{a_j}] = i\sum_{k=1}^{n} c_{ij}^k T_{a_k} \tag{3.106}$$

Then each element $a = \sum_{k=1}^{n}\alpha_k a_k$ of the Lie algebra is put into correspondence to the operator

$$T_a = \sum_{k=1}^{n}\alpha_k T_{a_k} \tag{3.107}$$

and conditions in eq. (3.98) are easily verified, that is, we obtain a representation of the Lie algebra g and, therefore, the Lie group G. Thus, the construction of representations of Lie group G in the space R reduces to construction of a set of operators $\{T_{a_k}\}$ satisfying given commutation relations.

This process is simplified when G is a *matrix* group. In this case, commutation relations are reduced to commutation relations for generators A_k of one-parameter subgroups a_k:

$$[A_i, A_j] = i\sum_{k=1}^{n} c_{ij}^k A_k \tag{3.108}$$

There is an exponential relation between the generators

$$A = \sum_{k=1}^{n}\alpha_k A_k \tag{3.109}$$

sufficiently close to zero and matrices of the Lie group G sufficiently close to the identity:

$$U = e^{-iA} = e^{-i\sum\limits_{k=1}^{n}\alpha_k A_k} \tag{3.110}$$

Let U belong to a one-parameter subgroup,

$$U_\alpha = e^{-i\alpha A} \tag{3.111}$$

with $\alpha = 1$. Then, according to eq. (3.99), the corresponding operators are

$$T_{U_\alpha} = e^{-i\alpha T_A} \tag{3.112}$$

(where a is replaced by generator A and operator T_a is replaced by operator T_A), and for $\alpha = 1$, we obtain the operator

$$T_U = e^{-iT_A} \tag{3.113}$$

Using eqs. (3.109) and (3.107), rewrite it as

$$T_U = e^{-i\sum\limits_{k=1}^{n} \alpha_k T_{A_k}} \tag{3.114}$$

Thus, we come to the following method to construct representations of matrix Lie groups:

(1) Basis matrix A_k of the Lie algebra is put in correspondence to Hermitian operators T_{A_k} in the space R with the same commutation relations.
(2) Matrices U of the Lie group sufficiently close to the identity are represented in the form (3.110).
(3) Operators T_U are constructed in the form (3.114) with the same coefficients α_k.

The following example will explain this. Suppose we want to build a two-dimensional representation of SO(3) group. The basis of the Lie algebra is composed in this case of matrices A_1, A_2, A_3 (eq. (3.36)) with commutation relations (eq. (3.75)). Consider matrices of the second order τ_1, τ_2, τ_3 (eq. (3.37)) with the same commutation relations (eq. (3.76)). Then, the representation of the Lie algebra is given by the rule

$$\text{If } A = \alpha_1 A_1 + \alpha_2 A_2 + \alpha_3 A_3, \quad \text{then } T_A = \alpha_1 \tau_1 + \alpha_2 \tau_2 + \alpha_3 \tau_3, \tag{3.115}$$

(where operators in a two-dimensional space are identified with their matrices), and the representation of SO(3) is given by the rule

$$\text{If } O = e^{-i(\alpha_1 A_1 + \alpha_2 A_2 + \alpha_3 A_3)}, \text{ then } T_O = e^{-i(\alpha_1 \tau_1 + \alpha_2 \tau_2 + \alpha_3 \tau_3)}. \tag{3.116}$$

To build a five-dimensional representation SO(3), take Hermitian matrices

$$T_{A_1} = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & \frac{\sqrt{6}}{2} & 0 & 0 \\ 0 & \frac{\sqrt{6}}{2} & 0 & \frac{\sqrt{6}}{2} & 0 \\ 0 & 0 & \frac{\sqrt{6}}{2} & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 \end{bmatrix}, \quad T_{A_2} = \begin{bmatrix} 0 & i & 0 & 0 & 0 \\ -i & 0 & \frac{\sqrt{6}}{2} i & 0 & 0 \\ 0 & -\frac{\sqrt{6}}{2} i & 0 & \frac{\sqrt{6}}{2} i & 0 \\ 0 & 0 & -\frac{\sqrt{6}}{2} i & 0 & i \\ 0 & 0 & 0 & -i & 0 \end{bmatrix},$$

$$T_{A_3} = \begin{bmatrix} -2 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 2 \end{bmatrix} \tag{3.117}$$

Evidently, they satisfy the same commutation relations as A_1, A_2, A_3. The formulas of the representations are similar to eqs. (3.115) and(3.116). As can be shown, the constructed representations of SO(3) are *irreducible*. Appendix B, Section 1 describes the method to construct irreducible representations of this group in the general case.

The following method is often useful when representations of Lie algebras are constructed. If the operators of the representation are already known, they can be used to construct linear combinations not only with real but also with complex coefficients; for example, for SO(3) group, the operators are

$$T_+ = T_{A_1} + iT_{A_2}, \quad T_- = T_{A_1} - iT_{A_2} \tag{3.118}$$

These operators can be important in physics; for example, in the representation $\{T_0\}$, eq.(3.118) can be used to obtain operators L_+, L_-, which rise or lower the projections of angular momentum L_3. To define such operators in all representations at once, consider as their preimages the complex linear combinations of the matrices of Lie algebra:

$$A_+ = A_1 + iA_2, \quad A_- = A_1 - iA_2 \tag{3.119}$$

Since Lie algebras allow multiplication only for *real* numbers, these matrices do not belong to the Lie algebra of SO(3). Further, nothing corresponds to such matrices in the representations of the Lie algebra, so Lie algebra and its representations are to be extended to construct operators (eq. (3.118)).

This is achieved as follows. Let g be any (matrix or nonmatrix) Lie algebra. All possible linear combinations $a + ib$ of elements a and b from g constitute a *complex envelope* of the Lie algebra g. These combinations are considered equal if and only if their "real" and "imaginary" parts are equal, that is, from $a + ib = c + id$, it follows that $a = c$, $b = d$. Thus, the transition from the Lie algebra to its complex envelope is similar to that from real to complex numbers. In this definition, the elements of the Lie algebra, that is, parameter subgroups, rather than their generators are considered.[30]

Operations in algebra g are applied to its complex envelope according to the following rules:

30 For matrix groups, it is not always possible to construct a complex envelope from the generators of the Lie algebra. For example, for the group GL(n,C), Lie algebra consists of *all* complex matrices; in this case, matrices A and iA are generators of some one-parameter subgroups, a and b, but in the complex envelope, by its definition, $b \neq ia$! Therefore, the complex envelope is constructed directly from the elements of the Lie algebra, that is, one-parameter subgroups, rather than from the generators. However, in the important case, when the Lie algebra consists of *Hermitian* matrices, this precaution is not essential since for a Hermitian matrix A, matrix iA is not Hermitian and thus does not belong to the Lie algebra. In this case, complex envelope can be constructed from the generators.

(1) $(a + ib) + (c + id) = (a + c) + i(b + d)$;

(2) $(\lambda + i\mu)(a + ib) = (\lambda a - \mu b) + i(\mu a + \lambda b)$ (where λ, μ are real numbers); (3.120)

(3) $[a + ib, c + id] = ([a, c] - [b, d]) + i([b, c] + [a, d])$.

From a given representation of Lie algebra g, the presentation of its complex envelope is constructed as follows:

$$\text{If } T_a,\ T_b \text{ represent } a,\ b,\ \text{ then } \ T_a + iT_b \text{ represents } \ a + ib\,.$$

As is easily seen, the properties of representation (3.98) are true when the elements of the Lie algebra change to the elements of its complex envelope.

In some cases, it is more convenient to choose a basis in the complex envelope of g and first construct representing operators for this basis and then for the elements of the Lie algebra and express them in terms of the "imaginary" basis. For example, for the group SO(3), such "imaginary" basis are matrices A_+, A_-, A_3 (see eq. (3.119)), with commutation relations:

$$[A_3, A_+] = A_+, \quad [A_3, A_-] = -A_-, \quad [A_+, A_-] = 2A_3 \tag{3.121}$$

If operators T_+, T_-, T_3 are constructed in R with commutation relations,

$$[T_3, T_+] = T_+, \quad [T_3, T_-] = -T_-, \quad [T_+, T_-] = 2T_3 \tag{3.122}$$

Then, expressing the basis of the Lie algebra in terms of the "imaginary basis,"

$$A_1 = \frac{1}{2}(A_+ + A_-), \quad A_2 = \frac{1}{2i}(A_+ - A_-), \quad A_3 = A_3 \tag{3.123}$$

define

$$T_{A_1} = \frac{1}{2}(T_+ + T_-), \quad T_{A_2} = \frac{1}{2i}(T_+ - T_-), \quad T_{A_3} = T_3 \tag{3.124}$$

These operators evidently satisfy the required commutation relations with the same structure constants as in eq. (3.75). Further, we will use the described technique.

Faithful representations of Lie groups make it possible to find commutation relations for nonmatrix Lie groups, because in these representations, the commutation of one-parameter subgroups reduces to the commutation of their generators, that is, to a simple algebraic operation of the form $AB–BA$ on the operators of the representation. Consider, for example, representation (3.25) of the isometry group. As is easily verified, the representation is faithful. Using such isomorphic model of the isometry group, find commutation relations for the group of operators (see eq. (3.98)) rather than the commutation relations for the group $M(3)$. For the rotations about axes x,y, the corresponding generators of the operator group have the form

$$T_1 = \frac{1}{i}\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right), \quad T_2 = \frac{1}{i}\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right). \tag{3.125}$$

Their commutator

$$\begin{aligned}\frac{1}{i}[T_1, T_2] &= -\frac{1}{i}\left\{\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right)\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right) - \left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right)\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right)\right\} \\ &= -\frac{1}{i}\left(y\frac{\partial}{\partial x} + yz\frac{\partial^2}{\partial z\partial x} - yx\frac{\partial^2}{\partial z^2} - z^2\frac{\partial^2}{\partial y\partial x} + zx\frac{\partial^2}{\partial y\partial z}\right. \\ &\qquad \left. - zy\frac{\partial^2}{\partial x\partial z} + z^2\frac{\partial^2}{\partial x\partial y} + xy\frac{\partial^2}{\partial z^2} - x\frac{\partial}{\partial y} - xz\frac{\partial^2}{\partial z\partial y}\right) \\ &= \frac{1}{i}\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) = T_3,\end{aligned} \tag{3.126}$$

which is equivalent to the relation $[A_1, A_2] = iA_3$ obtained directly for matrices (eq. (3.36)) of SO(3) subgroup.

For the translations along axis x, we have the operator $T_x = \frac{1}{i}\frac{\partial}{\partial x}$. The commutation relation for the generator of translation and the generator of rotation is now obtained by direct calculation similar to eq. (3.56):

$$\begin{aligned}\frac{1}{i}[T_x, T_3] &= \frac{1}{i}\left\{\frac{1}{i}\frac{\partial}{\partial x}\frac{1}{i}\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) - \frac{1}{i}\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)\frac{1}{i}\frac{\partial}{\partial x}\right\} \\ &= -\frac{1}{i}\left(\frac{\partial}{\partial y} + x\frac{\partial^2}{\partial x\partial y} - y\frac{\partial^2}{\partial x^2} - x\frac{\partial^2}{\partial y\partial x} + y\frac{\partial^2}{\partial x^2}\right) = -\frac{1}{i}\frac{\partial}{\partial y} = -T_y\end{aligned} \tag{3.127}$$

that is, $[T_x, T_3] = -iT_y$. The reader is encouraged to find all commutation relations for the basic generators T_1, T_2, T_3, T_x, T_y, T_z.

The method to construct representations of Lie groups with the help of their Lie algebras is, generally speaking, of local nature, that is, allows defining operators T_g only for the elements g sufficiently close to the identity. If, for example, in the case of a matrix group, matrix U can be expressed as e^{-iA} in various ways (see eq. (3.7)), the operator T_A and, consequently, e^{-iT_a} are not unique. For the group SO(3), irreducible global representations exist only in odd-dimensional spaces, while even-dimensional spaces contain only local representations, which results in the so-called "two-valued representations." In simple cases (see Chapters 1 and 2), the representations could be built "in large" without Lie algebras. In this book, we need only local representations, but "global" issues are important in some areas of physics.

3.4 Universal enveloping algebras and Casimir operators

As we saw in Chapter 2, Lie algebra provides "main observables" of the symmetry group: to find them, we need to find its representation in the space of the states of the physical system. This, however, does not cover all observables of interest for physics: for example, the Hamiltonians are constructed from the Casimir operators of the symmetry group and its subgroups which are *polynomials* of the representing operators. For many physical systems with different state spaces, the symmetry group is a subgroup of the isometry group. This was shown in Chapter 1 for spinless particles described by one-component wave functions; the same is true for the particles of any spin described by wave functions with any number of components. In all these cases, besides the operators of momentum p_x, p_y, p_z and angular momentum L_x, L_y, L_z constructed from one-parameter subgroups of the isometry group in the corresponding representations of its Lie algebra, there are other more complex observables such as the kinetic energy operator $\frac{1}{2m}p^2 = \frac{1}{2m}(p_x^2 + p_y^2 + p_z^2)$, the operator of "total angular momentum" $L^2 = L_x^2 + L_y^2 + L_z^2$, and so on. These operators are polynomials of the representing operators, and each type of polynomial, regardless of the representation, corresponds to the *same observable*. It is natural to construct such observables "in general", that is, consider "standard polynomials" of the elements of the Lie algebra which define the way of constructing observables in all representations. But here we meet an obstacle: in contrast to representing operators, the elements of the Lie algebra cannot be multiplied by each other. If we want to have a common preimage of energy or angular moment operators in various representations, we cannot achieve the goal within a Lie algebra. To find a clear algebraic meaning for the polynomials, we have to introduce a new concept.

First of all, it is convenient to have not only the preimages of one-parameter subgroups of operators (eq. (3.99)) in the Lie group but also their inverse images of generators T_A. For matrix groups, this role is played by generators of one-parameter subgroups of the Lie group itself: matrix subgroup $a = \{U_a\}$ belonging to the Lie algebra g is put in correspondence to matrix A according to eq. (3.23). In the general case, when this construction is not possible, we will denote each one-parameter subgroup of a Lie group $a = \{g_a\}$ with symbol A having no operator interpretation, which we will also call a *generator* of the one-parameter subgroup a. Also agree that operations on the elements of the Lie algebra correspond to the same operations on the generators, like it is in the matrix case (see eq. (3.51)):

$$\begin{aligned} &\text{If } c = a + b, \quad \text{then } C = A + B. \\ &\text{If } c = \lambda a, \quad \text{then } C = \lambda A \ (\lambda \text{ is a real number}). \\ &\text{If } c = [a, b], \quad \text{then } C = \tfrac{1}{i}[A, B]. \end{aligned} \tag{3.128}$$

The relations $[A, B] = iC$ where the elements of the Lie algebra are replaced by their generators are called *commutation relations in the algebra* g.

Preimages of the observables are polynomials of the generators of the Lie algebra g. Consider formal polynomials with complex coefficients $P(A, B, ...)$, $Q(A, B, ...)$, and so on. The expression "formal polynomial" means that its monomials such as $2AB$, $iABC$, and so on, are purely symbolical and serve as models to construct similar operator monomials in the representations $2T_AT_B$, $iT_AT_BT_C$, and so on. Further, for formal polynomials, in contrast to usual polynomials, the order of the factors is essential (so that, for example, the monomials ABC and ACB are considered different), but the order of the summands is indifferent. The agreement is adapted to operator representations of such polynomials as commutation is true for the addition but not for the multiplication. For formal polynomials, the operations of addition, multiplication by complex numbers, and multiplication by each other are defined. To add up polynomials P and Q, we should write down the polynomial P, put a plus sign, write down the polynomial Q, and collect similar monomials; that is, write down one monomial $(z_1 + z_2)AB \dots C$ instead of two monomials $z_1AB \dots C$, $z_2AB \dots C$ differing only by complex coefficients z_1, z_2 (if such exist). To multiply a polynomial P by number z, the coefficients of all monomials which are members of P should be multiplied by z. To multiply P by Q, we should for each monomial $z_1AB \dots C$ of P and for each monomial $z_2DE \dots F$ of Q write down the monomial $(z_1z_2)AB \dots CDE \dots F$ (keeping the order of the factors) to connect all such monomials by plus signs and to collect similar terms. It is easily verified that these operations make the set of all formal polynomials an *associative* algebra, that is, both the condition (3.61) and the condition $(PQ)R = P(QR)$ are met.

However, various formal polynomials $P(A, B, \dots)$, $Q(A, B, \dots)$ can correspond in *all* representations to the same operators $P(T_A, T_B, \dots)$, $Q(T_A, T_B, \dots)$. Namely, transformations of formal polynomials by the operations of the Lie algebra can be specified such that their images do not change in the representations:

(1) Let the polynomial P contains $AB \dots C \dots D$, where $C = C_1 + C_2$ in the Lie algebra g. Then P transforms into the polynomial Q containing the sum of two monomials $zAB \dots C_1 \dots D + zAB \dots C_2 \dots D$ instead of this monomial. Vice versa, Q transforms into P.

(2) Let the polynomial P contain the monomial $zAB \dots C \dots D$, where $C = \lambda C_1$ in g (λ is real). Then P transforms into the polynomial Q containing the monomial $(\lambda z)AB \dots C_1 \dots D$ instead of this monomial. Vice versa, Q transforms into P.

(3) Let the polynomial P contain the monomial $zAB \dots C \dots D$, where $iC = [C_1, C_2]$ in g. Then P transforms into the polynomial Q containing the sum of two monomials $\frac{z}{i}AB \dots C_1C_2 \dots D - \frac{z}{i}AB \dots C_2C_1 \dots D$ instead of this monomial. Vice versa, Q transforms into P.

Consider, for example, how transform (3.129) is imaged in representations. Polynomial P corresponds to the operator polynomial with monomial $zT_AT_B \dots T_C \dots T_D$. According to the definition of representations of the Lie algebra (3.98), commutation

relation $[C_1, C_2] = iC$ symbolizing the commutation relation $[c_1, c_2] = c$ in the Lie algebra, obtain $[T_{C_1}, T_{C_2}] = iT_C$ whence $zT_AT_B \dots T_C \dots T_D = \frac{z}{i}T_AT_B \dots T_{C_1}T_{C_2} \dots T_D - \frac{z}{i}T_AT_B \dots T_{C_2}T_{C_1} \dots T_D$.

But it is exactly this pair of monomials which is contained in Q.[31]

Polynomials $P(A, B, \dots)$ and $Q(A, B, \dots)$ are called *equivalent* if they can be transformed into each other by some number of operations (3.129). Since they correspond to the same operators in all representations, it is reasonable to identify such polynomials as a single object or an equivalence class. This procedure of considering mathematical objects "up to equivalence" is usual in mathematics (for example, in constructing factor groups). The equivalence class of formal polynomials is exactly the *observable of the symmetry group G* used to construct the operators of this observable in the representations of G, that is, for special physical systems. This general concept of the observable includes also the "main observables" defined above: in this case, we take classes containing polynomials of the first degree A, B, ..., that is, those corresponding to the elements of the Lie algebra. For equivalence classes, the same operations can be defined as for polynomials; if, for example, class $\widetilde{P}$ contains polynomial P and class $\widetilde{Q}$ contains polynomial Q, then the class containing $P + Q$ is called the sum $\widetilde{P} + \widetilde{Q}$; it does not depend on the choice of the "representatives" of P and Q in their equivalence classes. Multiplication of classes by complex numbers and by each other is similarly defined. The resulting associative algebra is called a *universal enveloping algebra* of the Lie algebra $\mathfrak{g}$ (or Lie group G); we denote it $\widetilde{\mathfrak{g}}$. This is the mathematical definition comprising all observables of the symmetry group G.

In practice, polynomials P, Q,... are considered up to equivalence, that is, equivalent polynomials are viewed as the same object (and are often combined by the equality sign). For example, for SO(3) group with generators A_k (k = 1,2,3), the polynomial $P(A_1, A_2, A_3) = A_1^2 + A_2^2 + A_3^2$ can be transformed using the commutation relation $[A_1, A_2] = iA_3$ into the equivalent polynomial $Q(A_1, A_2, A_3) = A_+A_- + A_3(A_3 - 1)$, where $A_\pm = A_1 \pm iA_2$. In any representation T, where $T_{A_k} = L_k$, the equivalence of P and Q leads to the *equality* of operators:

31 Note that in the case of a matrix group, different formal polynomials $P(A, B, \dots)$ and $Q(A, B, \dots)$ may coincide when symbolic generators are replaced by corresponding matrices. If, however, P and Q do not transform into each other according to eq. (3.129), such coinciding of matrices results in coinciding of operators only in the fundamental representation rather than in *all* representations. For example, we can construct a three-dimensional representation of SU(2) group defining a correspondence between basic matrices τ_k of the Lie algebra and matrices A_k (k = 1,2,3) (see eq. (3.115)) where, to the contrary, a two-dimensional representation of SO(3) was constructed. As is easily seen, $\tau_1^2 = \frac{1}{4}\sigma_1^2 = \frac{1}{4}$, so that polynomials $P(\tau_1, \tau_2, \tau_3) = \tau_1^2$ and $Q(\tau_1, \tau_2, \tau_3) = \frac{1}{4}$ (consisting of a free term only) correspond to the same second-order matrix. But in three-dimensional representation, we have

$$P(T_{\tau_1}, T_{\tau_2}, T_{\tau_3}) = A_1^2\begin{bmatrix}0 & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & 1\end{bmatrix}, \quad Q(T_{\tau_1}, T_{\tau_2}, T_{\tau_3}) = \begin{bmatrix}1/4 & 0 & 0\\ 0 & 1/4 & 0\\ 0 & 0 & 1/4\end{bmatrix} \tag{3.129}$$

$$L_1^2 + L_2^2 + L_3^2 = L_+L_- + L_3(L_3 - 1) \tag{3.130}$$

where $L_\pm = L_1 \pm iL_2$. This is a general equation for the projections of the angular momentum.

Sometimes in mathematical (and very often in physical) works, simplified designations of representing operators are used: $g, h, \ldots$ are written instead of $T_g, T_h, \ldots$; $A, B, \ldots$ are written instead of $T_A, T_B, \ldots$; and, similarly, $P(A, B, \ldots)$ is written instead of $P(T_A, T_B, \ldots)$.

Casimir *elements*, that is, the elements of $\tilde{\mathfrak{g}}$ which commute with all elements of $\tilde{\mathfrak{g}}$ are most important of all the elements of the universal enveloping algebra. (Mathematically, they form the *center* of algebra $\tilde{\mathfrak{g}}$.) Polynomial $P(A, B, \ldots)$ representing the Casimir element up to equivalence commutes with all generators $A,B,C,\ldots$ of $\mathfrak{g}$.

When verifying commutation relations, the so-called "second Jacobi identity" for associative algebras is helpful:

$$[C, AB] = [C, A]B + A[C, B]. \tag{3.131}$$

This identity is easy to remember by formal analogy with the rule for differentiating a product: commutator C with the product AB equals the sum of commutator C with the first factor multiplied by the second factor, and the first factor multiplied by commutator C with the second factor. The difference with the differentiation rules is that the order of the factors is essential in the case of commutation since multiplication of operators is not commutative. Verification of eq. (3.132) is simple:

$$\begin{aligned}[C, AB] &= C(AB) - (AB)C = (CAB - ACB) + (ACB - ABC) \\ &= (CA - AC)B + A(CB - BC) = [C, A]B + A[C, B]\end{aligned} \tag{3.132}$$

Similar to the rule for differentiating a product, the identity (eq. (3.132)) extends to any number of factors $A, B, \ldots$

Apply the rule (3.132) to the polynomial $A_1^2 + A_2^2 + A_3^2$ of the generators of SO(3):

$$\begin{aligned}[A_1, A_1^2 + A_2^2 + A_3^2] &= [A_1, A_1^2] + [A_1, A_2^2] + [A_1, A_3^2] \\ &= 0 + [A_1, A_2]A_2 + A_2[A_1, A_2] + [A_1, A_3]A_3 + A_3[A_1, A_3] \\ &= (iA_3)A_2 + A_2(iA_3) - (iA_2)A_3 - A_3(iA_2) = 0,\end{aligned} \tag{3.133}$$

and similarly for A_2, A_3. Consequently, the polynomial $A_1^2 + A_2^2 + A_3^2$ represents an element of the universal enveloping algebra of $SO(3)$, which is a Casimir element. Instead of these bulky expressions, we will say shorter: the polynomial $A_1^2 + A_2^2 + A_3^2$ is a *Casimir operator* of $SO(3)$ group. Of course, this way of speaking is conventional as *operators* are obtained from this polynomial only in the representations. In any representation where generator A_k is associated with operator L_k ($k = 1, 2, 3$), we obtain the Casimir operator $L_1^2 + L_2^2 + L_3^2$ denoted briefly L^2. In this designation, L^2 is considered as a single symbol: operator L is not defined (and if defined, it has an inconvenient expression).

The role of Casimir operators is that in some cases they make it possible to identify and describe irreducible representations. This process is based on Schur's lemma mentioned in Section 2.2. Now we formulate it again and prove it in the simplest case. Agree to use following term: if operator C is defined on space R so that $Cv = \lambda v$ for all vectors v from R and number λ does not depend on v, then the operator C is said to be constant on R and equal λ. (In mathematics, such operator is also called a *homothety*.) In other words, R is the proper space of operator C. Schur's lemma is formulated as follows.

Let an irreducible representation $\{T_g\}$ of group G be defined on the space R. If operator C defined on R commutes with all operators of T_g, then C is constant on R.

We prove this theorem only for finite-dimensional spaces. First, a preliminary statement will be proved:

In the conditions of the theorem, operator C is either identically zero or is nonzero for all vectors v.

Indeed, assume the contrary: let set R_0 of vectors v such that $Cv = 0$ is not reduced to the zero vector but differs from R. Then R_0 is a vector subspace: if v_1 and v_2 belong to R_0 ($Cv_1 = 0$, $Cv_2 = 0$), then $C(v_1 + v_2) = Cv_1 + Cv_2 = 0$ ($v_1 + v_2$ belongs to R_0), and if v belongs to R_0 ($Cv = 0$), then $C(\lambda v) = \lambda C(v) = 0$ (λv belongs to R_0). We will now prove that R_0 is an invariant subspace of representation $\{T_g\}$ which contradicts to the irreducibility of the representation. In fact, if v belongs to R_0, then $Cv = 0$, whence $T_g Cv = 0$ for all g; by the condition this is equivalent to $CT_g v = 0$, and this means that all vectors $T_g v$ belong to R_0. This contradiction proves our preliminary statement. Note that the same statement is true also for the operator $C - \lambda \cdot 1$ for any complex number λ; indeed, according to the conditions of the theorem, this operator commutes with all T_g.

Until now, we have not used the assumption about the finite dimensionality of R. In a finite-dimensional space, the equation $(C - \lambda \cdot 1)v = 0$ is equivalent to the homogeneous system of linear equations $\sum_{j=1}^{n}(c_{ij} - \lambda\delta_{ij})v_j = 0$ having a nonzero solution provided that that $det|c_{ij} - \lambda\delta_{ij}| = 0$. This is a so-called *secular equation*. As an algebraic equation, it has a complex root λ. For this λ, the equation $(C - \lambda \cdot 1)v = 0$ has a nonzero solution v; therefore, for the operator $C - \lambda \cdot 1$, the subspace R_0 is not reduced to the zero vector. From the above preliminary statement, we have $R_0 = R$, that is, $Cv = \lambda v$ for all v, and the operator C is constant.

Schur's lemma is usually applied in the following situation. Let C be a Casimir operator of group G (which is verified, for example, by the second Jacobi identity like it was done in eq. (3.134)). If representation $\{T_g\}$ (generally speaking, reducible) of group G is defined in the space R, then R decomposes into a sum of irreducible subspaces R_k. From Schur's lemma, operator C is constant on each R_k and takes some value λ_k. Assume that all numbers λ_k are different. Then the expansion of space R into irreducible subspaces amounts to finding eigensubspaces of the Casimir operator C, which are desired irreducible subspaces of R_k. The simplification is achieved due to the fact that instead of considering the behavior of vectors in R relative to the *group* of operators T_g, we can study their behavior under the action of a single

operator C. To better understand this method, consider again the examples discussed in Section 2.2.

If the values of the Casimir operator on irreducible subspaces are not all different, we should find all independent Casimir operators of group G. Denote them $C_1, ..., C_r$, and their values on the irreducible subspaces R_k as $\lambda_k^{(1)}, ..., \lambda_k^{(r)}$, respectively. In many cases, these sets of eigenvalues do not coincide for different k; then the complete system of Casimir operators makes it possible to identify all irreducible subspaces as eigensubspaces of the system of r commuting operators $C_1, ..., C_r$ and describe them by the above sets of eigenvalues. The same method is used to reduce irreducible representations of group G with respect to its subgroup G_1, for this goal, the Casimir operators of this subgroup are used.

3.5 Tensor product of representations

Consider now some methods to construct other groups and representations from Lie groups and their representations. Let G and H denote arbitrary groups; construct from them their *product* K. The elements of K are ordered pairs (g, h), where g is an element of G and h is an element of H; the multiplication of such pairs is done by the rule

$$(g_1, h_1) \cdot (g_2, h_2) = (g_1 g_2, h_1 h_2). \tag{3.134}$$

It is easily verified that this multiplication is associative, the identity in K is the pair (e_G, e_H), where e_G is the identity in G, e_H is the identity in H, and (g^{-1}, h^{-1}) is the inverse element to (g, h). Therefore, K is a group. The group is called the *product* of groups G, H, respectively, and is designated $G \times H$. Group K contains a subgroup consisting of elements (g, e_H) which are multiplied the same way as their first factors in G; this subgroup is therefore isomorphic to G. Denote it $G \times 1$. Similarly subgroup $1 \times H$ consisting of elements (e_G, h) is constructed; it is isomorphic to H.

Evidently, each element from K uniquely decomposes into a product of elements from $G \times 1$ and $1 \times H$: $(g, h) = (g, e_H)(e_G, h)$.

Further, from eq. (3.135), it follows that elements of $G \times 1$ commute with elements of $1 \times H$: $(g, e_H)(e_G, h) = (g, h) = (e_G, h)(g, e_H)$.

This situation can take place within some *given* group K. Assume that K contains commuting subgroups G, H; that is, $gh = hg$ for all elements g from G and h from H, and each element of K uniquely decomposes into a product of an element of G and an element of H: $k = gh$. Then, writing down k as (g, h), we can easily verify that pairs (g, h) are multiplied by the rule (3.135): from the commutativity of G and H, obtain

$$(g_1, h_1) \cdot (g_2, h_2) = (g_1 h_1) \cdot (g_2 h_2) = (g_1 g_2) \cdot (h_1 h_2) = (g_1 g_2, h_1 h_2). \tag{3.135}$$

Thus, in the above conditions, group K is isomorphic to the product of groups $G \times H$.

If G and H are Lie groups with dimensions d_G and d_H, respectively, then an element from G is described by d_G parameters, an element from H by d_H parameters and,

therefore, the pair (g, h) is described by $d_G + d_H$ parameters; thus, the dimension of $G \times H$ is $d_G + d_H$.

The definition of the product of groups is easily generalized for any number of factors: the elements of the product are sets $(g_1, \ldots, g_n)$ where g_k belongs to $G_k (k = 1, \ldots, n)$, and multiplication of such elements is performed by the rule:

$$(g_1, \ldots, g_n)\cdot(g'_1, \ldots, g'_n) = (g_1 g', \ldots, g_n g'_n). \tag{3.136}$$

In particular, if all G_k are isomorphic to the group of real numbers R^1 (with the operation of addition), then the product R^n is called an n-dimensional vector group; this operation in R^n is usually written additively (with the sign +). Another example is multiplication of n circles (a circle here is considered as a group of rotations of the plane $\mathrm{SO}(2)$). This product T^n is called an n-dimensional torus. In both examples, we obtain abelian (i.e. commutative) groups. It can be verified that each abelian Lie group is isomorphic either to R^m or to T^n or to the product $R^m \times T^n$. A more interesting example will be discussed in Section 5.2, where a nonabelian group $\mathrm{SO}(4)$ will be locally (in the vicinity of the identity) decomposed into a product of two copies of group $\mathrm{SO}(3)$.

Let representations $\{T_g\}, \{T_h\}$ of groups G, H, respectively, be defined in spaces $\mathsf{R}_1, \mathsf{R}_2$. Physically, it means that two quantum systems with state spaces $\mathsf{R}_1, \mathsf{R}_2$ and symmetry groups G, H are defined. If these systems constitute together some complex system, then the state of the latter is denoted $v \otimes w$, where v and w are state vectors of the first and the second systems, respectively. Linear combinations of such conditions also describe the states of the complex system (when the states of these both parts are not defined).

Mathematically, the state space of a complex system is constructed as follows. For Hilbert spaces $\mathsf{R}_1, \mathsf{R}_2$ there exists (up to isomorphism) such Hilbert space R, that are as follows:

(1) Each pair of vectors v from R_1 and w from R_2 corresponds to the vector $v \otimes w$ from R, such that

$$\begin{aligned} &(v_1 + v_2) \otimes w = v_1 \otimes w + v_2 \otimes w \\ &v \otimes (w_1 + w_2) = v \otimes w_1 + v \otimes w_2 \\ &(\lambda v) \otimes w = v \otimes \lambda w = \lambda (v \otimes w) \end{aligned} \tag{3.137}$$

(λ is a complex number).

(2) Each vector from R can be represented as $v_1 \otimes w_1 + v_2 \otimes w_2 + \ldots$, where the sum is finite if $\mathsf{R}_1, \mathsf{R}_2$ are finite, and, in general, is the sum of a series converging in the norm.

(3) The scalar product in R is defined as

$$\langle v_1 \otimes w_1 | v_2 \otimes w_2 \rangle_R = \langle v_1 | v_2 \rangle_R + \langle w_1 | w_2 \rangle_R, \tag{3.138}$$

where the first scalar product on the right side is taken in R_1, and the second in R_2.

The space R satisfying the above conditions is called the *tensor product* of spaces $\mathsf{R}_1, \mathsf{R}_2$.

In Physics, often the following simple method to construct the tensor product is used. Orthonormal bases $|\sigma\rangle$ and $|\tau\rangle$ are chosen in R_1 and R_2, respectively; the bases are numerated by numbers σ, τ, and each pair of vectors $|\sigma\rangle, |\tau\rangle$ is associated with an object called vector $|\sigma, \tau\rangle$; linear combinations of such vectors constitute the desired space R, and its basis vectors $|\sigma, \tau\rangle$ are implied normalized and orthogonal to each other. If $\mathsf{R}_1, \mathsf{R}_2$ have finite dimensions m,n, then R is also finite-dimensional and has dimension mn. The pair of vectors $v = \sum_\sigma \lambda_\sigma |\sigma\rangle$, $w = \sum_\tau \mu_\tau |\tau\rangle$ belonging to the spaces $\mathsf{R}_1, \mathsf{R}_2$, respectively, is associated with the vector

$$v \otimes w = \sum_{\sigma,\tau} \lambda_\sigma \mu_\tau |\sigma, \tau\rangle \tag{3.139}$$

from R.

Let $\{T_g\}$ be the representation of group G in the space R_1 and $\{T_h\}$ be the representation of group H in the space R_2. From these representations, some representation $\{T_k\}$ of group $K = G \times H$ is constructed in the space $\mathsf{R} = \mathsf{R}_1 \otimes \mathsf{R}_2$. Since the representation must be linear, it suffices to define operators T_k for vectors $v \otimes w$ because their sums constitute the whole space R. Define for the element $k = (g, h)$,

$$T_k(v \otimes w) = (T_g v) \otimes (T_h w). \tag{3.140}$$

Physically, it means that groups G, H act separately on the state vectors v, w of the subsystems, so that $G \times H$ is the symmetry group of the complex system. In particular, for the basis vectors, we have

$$T_k|\sigma, \tau\rangle = T_g|\sigma\rangle \otimes T_h|\tau\rangle. \tag{3.141}$$

If representations $\{T_g\}, \{T_h\}$ are irreducible, the representation $\{T_k\}$ can also be shown to be irreducible.

It is easily verified that if representations $\{T_g\}, \{T_h\}$ are unitary, then $\{T_k\}$ is also unitary. From eqs. (3.141) and (3.139),

$$\begin{aligned} \langle T_k(v_1 \otimes w_1)|T_k(v_2 \otimes w_2)\rangle &= \langle (T_g v_1) \otimes (T_h w_1)|(T_g v_2) \otimes (T_h w_2)\rangle \\ &= \langle T_g v_1|T_h w_1\rangle + \langle T_g v_2|T_h w_2\rangle, \end{aligned} \tag{3.142}$$

where scalar products on the right are taken in $\mathsf{R}_1, \mathsf{R}_2$, and since $\{T_g\}, \{T_h\}$ are unitary, obtain for the right side

$$\langle v_1|w_1\rangle + \langle v_2|w_2\rangle = \langle v_1 \otimes w_1|v_2 \otimes w_2\rangle. \tag{3.143}$$

Especially important is the case when one of the groups, for example, G, is the SU(2) group, and representation $\{T_g\}$ is a fundamental representation of this group in the two-dimensional complex space C^2. In this case, index σ takes two values usually chosen as $-\frac{1}{2}$ and $\frac{1}{2}$; then the basis of the space R consists of vectors $|\sigma, \tau\rangle$, and for $\sigma = -\frac{1}{2}$ and $\sigma = \frac{1}{2}$, obtain subspaces $\mathsf{R}^+, \mathsf{R}^-$, respectively, generated by vectors $|-\frac{1}{2}, \tau\rangle$, $|\frac{1}{2}, \tau\rangle$, and in each of them, a representation of group H is defined. The representations $\{T_h^-\}, \{T_h^+\}$ act only on number τ and do not change σ.

As can be verified, one-parameter subgroups $\{g_\alpha, 1\}, \{1, h_\alpha\}$ belonging to G and H together form a complete set of generators of the Lie algebra of group K. In the space R of the representation $\{T_k\}$, one-parameter subgroups G correspond to operators A_G acting only on the number σ, that is, transforming basis vectors $|\sigma, \tau\rangle$ into linear combinations of vectors with the same τ; similarly, one-parameter subgroups H correspond to operators A_H acting only on the number τ. In particular, for $G = \mathrm{SU}(2)$ and fundamental representation $\{T_g\}$, operators A_g are reduced to matrices $\tau_k = \frac{1}{2}\sigma_k$ and their linear combinations which transform components $|-\frac{1}{2}, \tau\rangle, |\frac{1}{2}, \tau\rangle$. Denoting $\tau_+ = \tau_1 + i\tau_2$, $\tau_- = \tau_1 - i\tau_2$, we have

$$\tau_+\left|-\frac{1}{2}, \tau\right\rangle = \left|\frac{1}{2}, \tau\right\rangle, \quad \tau_-\left|\frac{1}{2}, \tau\right\rangle = \left|-\frac{1}{2}, \tau\right\rangle, \quad \tau_3|\sigma, \tau\rangle = \sigma|\sigma, \tau\rangle\left(\sigma = \mp\frac{1}{2}\right). \quad (3.144)$$

Consider now the case of isomorphic groups G, H. Then each element g from G corresponds to the element $\varphi(g)$ from H, where φ is an isomorphism. If H is assumed the second copy of the group G, we can for simplicity designate $\varphi(g)$ as g keeping in mind which factor the element belongs to. Then from two representations $\{T_g^{(1)}\}, \{T_g^{(2)}\}$ of group G in spaces $\mathsf{R}_1, \mathsf{R}_2$, respectively, a representation $\{T_g\}$ of *the same* group G in the space $\mathsf{R} = \mathsf{R}_1 \otimes \mathsf{R}_2$ can be constructed by the formula

$$T_g(v \otimes w) = (T_g v) \otimes (T_g w). \quad (3.145)$$

This representation is called a *tensor product* of representations $T^{(1)}$, $T^{(2)}$ and is denoted as

$$T = T^{(1)} \otimes T^{(2)}. \quad (3.146)$$

In contrast to the representation of $G \times H$ where the elements g and h vary independently (see eq. (3.141)), irreducible representations $T^{(1)}$, $T^{(2)}$ of group G usually makes it possible to obtain *reducible* representation T of group G. Expansion into irreducible representations $T = T^{(1)} \otimes T^{(2)}$ is the so-called Clebsch–Gordan problem.

A one-parameter subgroup $\{g_\alpha\}$ of group G corresponds in the representation T the subgroup of operators

$$T_{g_\alpha}(v \otimes w) = T_{g_\alpha}(v) \otimes T_{g_\alpha}(w). \quad (3.147)$$

By differentiating with respect to α, obtain the operators of the Lie algebra in the representation T:

$$i\frac{d}{d\alpha}T_{g_\alpha}(v \otimes w)|_{\alpha=0} = i\frac{d}{d\alpha}(T_{g_\alpha}(v) \otimes T_{g_\alpha}(w))|_{\alpha=0}. \quad (3.148)$$

The rule for differentiating a tensor product is derived the same way as for usual differentiation, and from eq. (3.149), obtain the operator corresponding to the generator of the subgroup $\{g_\alpha\}$ in the representation T:

$$i\frac{d}{d\alpha}T_{g_\alpha}(v)|_{\alpha=0} \otimes T_{g_0}(w) + iT_{g_0}(v) \otimes \frac{d}{d\alpha}T_{g_\alpha}(w)|_{\alpha=0} = A_1 v \otimes w + v \otimes A_2 w, \quad (3.149)$$

where A_1, *and* A_2 are the generators of the subgroup $\{g_\alpha\}$ in the representations $T^{(1)}$ and $T^{(2)}$, respectively. In particular, the operators of the Lie algebra act on the basis vectors $|\sigma, \tau\rangle$ as follows:

$$A|\sigma, \tau\rangle = A_1|\sigma\rangle \otimes |\tau\rangle + |\sigma\rangle \otimes A_2|\tau\rangle. \tag{3.150}$$

Having in mind the action of operators A_1 *and* A_2 described in eq. (3.151), we can write briefly

$$A = A_1 + A_2 \tag{3.151}$$

where operators A_1, A_2, A represent the generators of the corresponding one-parameter subgroups G, H, K.

In view of the isomorphism φ, the pairs $(g, \varphi(g))$ constitute in $G \times H$ a subgroup $\widetilde{G}$ which is also isomorphic to G, because the law of multiplicating pairs

$$(g_1, \varphi(g_1)) \cdot (g_2, \varphi(g_2)) = (g_1 g_2, \varphi(g_1)\varphi(g_2)) = (g_1 g_2, \varphi(g_1 g_2)) \tag{3.152}$$

is exactly the same as in G. Therefore, we can consider the tensor product of representations defined by eq. (3.146) as a presentation of the constructed subgroup $\widetilde{G}$ (rather than the first factor of $G \times H$).

Consider, for example, groups $G = \mathrm{SO}(3)$ and $H = \mathrm{SU}(2)$ with generators A_k and τ_k ($k = 1, 2, 3$), respectively. Then the correspondence $A_k \to \tau_k$ defines an isomorphism of Lie algebras, and the equation

$$\varphi\left(e^{-i\sum_{k=1}^{3}\alpha_k A_k}\right) = e^{-i\sum_{k=1}^{3}\alpha_k \tau_k} \tag{3.153}$$

defines the local isomorphism of G and H (i.e. isomorphic mapping connecting the vicinities of the identities of these groups). From two given representations $\{T_g\}, \{T_h\}$ of groups SO(3), SU(2), their tensor product can be constructed which is a local representation of $\widetilde{G}$ with elements $(O^{(3)}, \varphi(O^{(3)}))$.

4 The principles of particle classification

4.1 The concept of spin

Spin is an "internal degree of freedom" of the electron and has no classical analog. To describe the spin, in 1926, Pauli suggested representing electron states by *two-component* wave functions:

$$\psi = \begin{bmatrix} \psi_1(x,y,z) \\ \psi_2(x,y,z) \end{bmatrix}. \tag{4.1}$$

The summation of state vectors ψ and their multiplication by complex numbers are component-wise:

$$\psi + \varphi = \begin{bmatrix} \psi_1(x,y,z) + \varphi_1(x,y,z) \\ \psi_2(x,y,z) + \varphi_2(x,y,z) \end{bmatrix}, \ \lambda\psi = \begin{bmatrix} \lambda\psi_1(x,y,z) \\ \lambda\psi_2(x,y,z) \end{bmatrix}, \tag{4.2}$$

and their scalar product is defined as

$$\langle\psi|\varphi\rangle = \int (\psi^*{}_1\varphi_1 + \psi^*{}_2\varphi_2) d^3x. \tag{4.3}$$

Vector ψ is said to be normalized if $\|\psi\| = \sqrt{\langle\psi|\psi\rangle} = 1$. Transition probabilities between normalized vectors ψ and φ are $|\langle\psi|\varphi\rangle|^2$. If the state of an electron is defined by a normalized two-component wave function ψ, the probability to find the electron in the region D is

$$\int_D (|\psi_1|^2 + |\psi_2|^2) d^3x. \tag{4.4}$$

Thus, electron-spin states are described (in the nonrelativistic theory) by two-component wave functions ψ to constitute a Hilbert space. Designate this space $\mathbb{R}^2$.

As we saw, rotation group SO(3) is important in Schrödinger's zero-spin quantum mechanics. It is natural to expect that this group acts also in the space $\mathbb{R}^2$ of spin wave functions. To find the corresponding representation, we will use the analogy between two-component functions (4.34) and vector fields such as velocity field $v(x,y,z)$ and force field $F(x,y,z)$. Change of coordinates transforms the vector field the way that it is described in both systems by the same mathematical procedure to ensure the equality of all coordinate systems. The observer in the "old" coordinate system assigns coordinates x, y, z to point r and projects the vector field $v(r)$ at this point on the axes of the "old" system to obtain the components of the field $v_i(x,y,z)$ (i = 1,2,3). The observer in the "new" coordinate system assigns coordinates x', y', z' to the same point r and projects the same vector field $v(r)$ on the "new" axes to obtain the components of the field $v_i'(x',y',z')$. The new coordinates are expressed in terms of the old

coordinates by the orthogonal transformation $x' = Ox$, and so do new components of the field with respect to old components:

$$v_i'(x', y', z') = \sum_{j=1}^{3} o_{ij} v_j(x, y, z) \quad (i = 1, 2, 3) \tag{4.5}$$

Replacing x' by x, obtain

$$v_i'(x) = \sum_{j=1}^{3} o_{ij} v_j(O^{-1}x) \quad (i = 1, 2, 3) \tag{4.6}$$

The same transform results from the "active" interpretation with constant coordinate system and the whole field rotating; the reader is encouraged to verify this statement.

If the two-component wave function (4.1) is considered as an analog of a vector field, its transformation under rotation O is natural to search similar to eq. (4.6):

$$\psi'_\sigma(x) = \sum_{\tau=1}^{2} u_{\sigma\tau} \psi_\tau(O^{-1}x) \tag{4.7}$$

where $u = (u_{\sigma\tau})$ is the second-order matrix corresponding to O. Suppose that two rotations O_1 and O_2 act consecutively. Let $u^{(1)}$ and $u^{(2)}$ denote the corresponding matrices, then from eq. (4.7), obtain:

$$\psi''_\sigma(x) = \sum_{\tau=1}^{2} u^{(2)}_{\sigma\tau} \psi'_\tau(O_2^{-1}x), \quad \psi'_\tau(x) = \sum_{\rho=1}^{2} u^{(1)}_{\tau\rho} \psi_\rho(O_1^{-1}x) \tag{4.8}$$

Replacing x by $O_2^{-1}x$ in the second equation of eq. (4.8) and substituting $\psi'_\tau(O_2^{-1}x)$ in the first equation, we have

$$\psi''_\sigma(x) = \sum_{\tau=1}^{2} u^{(2)}_{\sigma\tau} \sum_{\rho=1}^{2} u^{(1)}_{\tau\rho} \psi_\rho(O_1^{-1}O_2^{-1}x) = \sum_{\rho=1}^{2} (u^{(2)}u^{(1)})_{\sigma\rho} \psi_\rho((O_1O_2)^{-1}x) \tag{4.9}$$

Therefore, the result of both transforms O_2, O_1 also has the form (4.7), and rotation O_1O_2 corresponds to the product of matrices $u^{(1)}u^{(2)}$ taken in the same order. It is natural to assume that the identity rotation $O = 1$ corresponds to the identity transformation $\psi' = \psi$, that is, the identity matrix u. This means that matrices $u = u_0$ corresponding to all possible rotations should constitute a *two-dimensional representation* of SO(3) group. If the transition probabilities, that is, scalar products (eq. (4.3)) are to be conserved, the representation should be *unitary*. In fact

$$\begin{aligned} \langle \psi' | \varphi' \rangle &= \int \sum_{\sigma=1}^{2} \psi'^{*}_\sigma(x) \varphi_\sigma(x) d^3x = \int \sum_{\sigma=1}^{2} \left(\sum_{\tau=1}^{2} u_{\sigma\tau} \psi_\tau(O^{-1}x) \right)^* \left(\sum_{\rho=1}^{2} u_{\sigma\rho} \varphi_\rho(O^{-1}x) \right) d^3x \\ &= \int \sum_{\tau,\rho=1}^{2} \left(\sum_{\sigma=1}^{2} u^*_{\sigma\tau} u_{\sigma\rho} \right) \psi^*_\tau(O^{-1}x) \varphi_\rho(O^{-1}x) d^3x = \int \sum_{\tau,\rho=1}^{2} ({}^t u^* u)_{\tau\rho} \psi^*_\tau(x) \varphi_\rho(x) d^3x \end{aligned} \tag{4.10}$$

(see the proof (1.20)). On the other hand,

$$\langle \psi | \varphi \rangle = \int \sum_{\tau=1}^{2} \psi_\tau^*(x) \varphi_\tau(x) d^3x.$$

To make it equal to eq. (4.10), the condition $({}^t u^* u)_{\tau\rho} = \delta_{\tau\rho}$, that is, ${}^t u^* = u^{-1}$ should be satisfied, which means that matrix u is unitary.

Thus, to find the rotation transformation of two-component wave functions, a two-dimensional unitary representation of SO(3) is to be found. It turns out that, up to equivalence, there are only two such representations: the identity representation and the irreducible representation described below. Under the identity representation ($u_0 = 1$), the components ψ_1, ψ_2 are transformed separately according to eq. (4.9); this provides no new results as compared to the spinless Schrödinger's theory. As we will see, the additional angular momentum of the electron, which initially was explained as a "rotation about its own axis," is correctly described by some irreducible representation.

To construct the representation, use the method described in Section 3.3. The basis of Lie algebra of SO(3) consists of three matrices A_κ (eq. (3.36)) satisfying commutation relations (eq. (3.75)). Each of them should be put into correspondence to the operator acting in a two-dimensional complex space or, in the chosen basis, to the second order matrix, so that these matrices obey the same commutation relations. Pauli matrices $\tau_k = \frac{1}{2}\sigma_k \quad (k = 1, 2, 3)$ multiplied by $\frac{1}{2}$ can be taken for this goal. Then the desired representation of the Lie algebra of SO(3) group is given by eq. (3.115), and the corresponding representation of SO(3) group is given by eq. (3.116). One-parameter subgroup of rotations about z axis

$$\begin{aligned} x' &= x\cos\alpha - y\sin\alpha \\ y' &= x\sin\alpha + y\cos\alpha \\ z' &= z \end{aligned} \tag{4.11}$$

corresponds to the subgroup of matrices

$$u_\alpha = e^{-i\alpha\tau_3} = e^{-i\alpha\frac{\sigma_3}{2}} \tag{4.12}$$

(see eq. (3.38)). One-parameter matrix subgroups corresponding to rotations about x, y are constructed in a similar way. Since matrices τ_k are Hermitian and traceless, the obtained representation is unitary, and the determinant of its matrices is 1.

The representation is irreducible. In fact, since operators of the representation of the Lie algebra are obtained as linear combinations of the representing operators of the group and by passage to the limit (see eq. (3.97)), an invariant subspace of the Lie group is also invariant for its Lie algebra. If C' is an invariant subspace of C^2 containing a nonzero vector $\begin{bmatrix} z_1 \\ z_2 \end{bmatrix}$, then, without loss of generality, assume that $z_1 \neq 0$ (otherwise it suffices to take, instead of $\begin{bmatrix} z_1 \\ z_2 \end{bmatrix}$, vector $\begin{bmatrix} z_2 \\ z_1 \end{bmatrix} = \sigma_1 \begin{bmatrix} z_1 \\ z_2 \end{bmatrix}$ also belonging to C').

Since $\begin{bmatrix} 2z_1 \\ 0 \end{bmatrix} = \begin{bmatrix} z_1 \\ z_2 \end{bmatrix} + \sigma_3 \begin{bmatrix} z_1 \\ z_2 \end{bmatrix}$ belongs to C' together with $\begin{bmatrix} z_1 \\ z_2 \end{bmatrix}$, C' contains all vectors $\begin{bmatrix} w \\ 0 \end{bmatrix}$, where w is any complex number. Similarly, it can be proved that C' contains all vectors $\begin{bmatrix} w \\ 0 \end{bmatrix}$; but then C' coincides with C^2.

Consider now the transformation law of two-component wave functions (eq. (4.7)). Replacing u by the matrix of representation u_O on the right side of eq. (4.7), from eq. (4.9), it follows that eq. (4.7) defines the representation of SO(3) in the space of two-component wavefunctions R^2. From eq. (4.10), it follows that the representation is unitary; designate it $\{T_O^{(2)}\}$.

Replacing O in eq. (4.12) by rotation (eq. (4.11)) and u by matrix (eq. (4.12)), obtain a one-parameter subgroup of operators $\{T_{O_\alpha}^{(2)}\}$ to transform ψ into ψ'_α:

$$\begin{aligned} (\psi'_\alpha)_1 &= e^{\frac{-i\alpha}{2}} \psi_1(x\cos\alpha + y\sin\alpha, -x\sin\alpha + y\cos\alpha, z), \\ (\psi'_\alpha)_2 &= e^{\frac{i\alpha}{2}} \psi_2(x\cos\alpha + y\sin\alpha, -x\sin\alpha + y\cos\alpha, z) \end{aligned} \tag{4.13}$$

Find the observable corresponding to this subgroup (see eq. (2.15)):

$$\lim_{\alpha\to 0} \frac{T_\alpha\psi - \psi}{\alpha} = \frac{d}{d\alpha}(T_\alpha\psi)|_{\alpha=0} = -\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)\begin{bmatrix}\psi_1 \\ \psi_2\end{bmatrix} - \frac{i}{2}\begin{bmatrix}1 & 0 \\ 0 & 1\end{bmatrix}\begin{bmatrix}\psi_1 \\ \psi_2\end{bmatrix} \tag{4.14}$$

Multiplying both sides by $i\hbar$, obtained is the Hermitian operator:

$$I_z\psi = \frac{\hbar}{i}\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)\psi + \frac{\hbar}{2}\sigma_3\psi \tag{4.15}$$

The first term in eq. (4.15) is the operator of the orbital angular momentum L_z, the same as in Schrödinger's one-component theory; it is applied to each component separately. The second term, designated S_z, is the electron-spin momentum which is a linear matrix operator to transform the components of the ψ function. Similarly, obtained formulas for I_x, I_y containing the operators of spin angular momentum $S_x = \frac{\hbar}{2}\sigma_1$ and $S_y = \frac{\hbar}{2}\sigma_2$. "Spin projections" are new observables of the Pauli's two-component theory. The form of these operators is confirmed experimentally as the observed values of angular momentum are the eigenvalues of $I = L + S$. If the spin can be neglected, then one-component Schrödinger theory is applicable, and the operators of the angular momentum are reduced to L. The above derivation of the operators of the electron's total angular momentum is close to the original Pauli's reasoning (see Pauli, 2000).

The operator of the projection of the spin momentum S_z has eigenvalues $\pm\frac{\hbar}{2}$ corresponding to the eigenvalues ± 1 of matrix σ_3. Eigenfunctions S_z are $\begin{bmatrix}\psi_1 \\ 0\end{bmatrix}$ and $\begin{bmatrix}0 \\ \psi_2\end{bmatrix}$. S_x and S_y have the same eigenvalues; the reader is encouraged to exercise in finding

their eigenfunctions. Matrices σ_k are chosen the way that σ_3, which corresponds to rotations about axis z, has the simplest diagonal view. This can simplify the tasks where axis z is oriented in the direction of the external field as is done when considering Zeeman and Stark effects. As follows from eq. (3.76), operator $S^2 = S_x^2 + S_y^2 + S_z^2$ commutes with the operators of spin angular momentum S_x, S_y, S_z; obviously, it commutes also with L_x, L_y, L_z and, therefore, with representing operators I_x, I_y, I_z of the Lie algebra of SO(3) group. From Schur's lemma, operator S^2 is constant on R^2; its value is found by taking any vector from R^2, for example, $\begin{bmatrix}\psi_1\\0\end{bmatrix}$. After simple calculations obtain $S^2 = \frac{1}{2}(\frac{1}{2}+1)\hbar^2 = \frac{3}{4}\hbar^2$. The largest eigenvalue of the operators of spin angular momentum S_x, S_y, S_z divided by ħ, that is, $\frac{1}{2}$, is called the *spin* of the electron. Operator S^2 is expressed in terms of the spin the same way as L^2 is expressed in terms of l. Note that operator S is not considered, so that S^2 should be viewed as a single symbol.

Pauli extended his theory to the particles with any spin. If, instead of two-component wave functions, d-component wave functions are taken, where d is any non-negative number, the above constructions can be repeated if matrices τ_k are replaced by matrices s_k ($k = 1, 2, 3$) of order d with the same commutation relations. This way, a d-dimensional irreducible unitary representation of SO(3) defined in a neighborhood of identity is obtained. Using the matrices of this representation u_O, a representation of SO(3) in the space of d-component wave functions can be constructed similar to eq. (4.7) and operators of total angular momentum similar to eq. (4.15). It can be shown that eigenvalues of spin operators s_k are $-s, -(s-1), \ldots, s-1, s$, where s is such that $d = 2s + 1$; therefore, s is an integer or a half-integer number, that is, $s = 0, 1/2, 1, 3/2, 2, \ldots$. Number s called the spin of the particle described by a d-component wave function. Operators of the spin momentum of such particle are related to spin operators as $S = \hbar s$. The value of the Casimir operator $S_x^2 + S_y^2 + S_z^2$ for a particle with spin s is $s(s+1)\hbar^2$.

Note that the method of constructing representations using Lie algebras ensures their uniqueness only in the neighborhood of the identity of the represented group. It can be shown that in odd-dimensional spaces, there exists a unique irreducible representation of the *whole* SO(3) group, and in even-dimensional spaces, there is only local representation. Appendix B contains a brief description of irreducible representations of SO(3) group.

4.2 Isotopic spin

In 1934, Heisenberg applied the concept of spin to describe protons and neutrons. In Pauli's (and Dirac's) theory of electron, different spin states of the electron are associated with the same particle because the electron in all spin states has the same

weight and charge and all these states obey the same equation of motion.[32] The proton and neutron have very close, though different, masses (938.3 and 939.5 MeV, respectively) and, indeed, different charges (+1 and 0). Heisenberg proposed to consider these two particles as different states of the same quantum system by analogy with spin states of the electron where $S_z = \pm \frac{\hbar}{2}$. The mass "splitting" is explained by analogy with energy levels splitting in magnetic fields, where the charge plays the role similar to the spin momentum.

The theory considers only spin states of a quantum system rather than its space–time behavior. In a sense, this approach is opposite to that discussed in Section 1.1, where the spin was neglected. Quantum mechanics can be constructed at different levels of description: relativistic and nonrelativistic; spin and spinless. Now we want to construct a *quantum mechanics of the spin*. The term will be justified the resulting theory has all characteristics of a quantum-mechanical description. We will call this system a "two-component spin."

Consider a two-dimensional complex space C^2 with two-component complex vectors z called *spinors* and designated as columns:

$$z = \begin{bmatrix} z_1 \\ z_2 \end{bmatrix}. \tag{4.16}$$

Comparing this record with two-component wave functions from Section 4.1, the spinor is assumed to provide the information about the spin of the electron, as z_1, z_2 do not depend on the coordinates or on the time. As we will see, such description of the spin is useful because it allows applying this concept to the other kind of problems. Define a scalar product in the space C^2,

$$\langle z|w\rangle = z_1^* w_1 + z_2^* w_2 \tag{4.17}$$

Thereby C^2 becomes a two-dimensional Hilbert space.[33] This will be the state space of our system with state vectors represented by non-zero spinors (eq. (4.16)). We will use orthonormal bases in C^2 such as, for example, a pair of spinors

$$e_1 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad e_2 = \begin{bmatrix} 0 \\ 1 \end{bmatrix}. \tag{4.18}$$

Take SU(2) as the symmetry group of the system. Therefore, the representation of the rotation group is no more used, because no spatial aspect of the system is considered;

32 A deeper reason of viewing the "electron with spin ½" and the "electron with spin −½" as the states of the same particle rather than two different particles is that the electron is described by the irreducible representations of the Poincare group which explain its spin (see, e.g. Rumer and Fet, 1977).
33 Often Hilbert spaces are assumed to be infinite-dimensional spaces with scalar product; we will not introduce another term for the finite-dimensional case.

unitary unimodular matrices u no longer represent rotations, rather they represent themselves, or, in the chosen basis of C^2, linear transforms

$$\begin{aligned} z_1' &= u_{11}z_1 + u_{12}z_2 \\ z_2' &= u_{21}z_1 + u_{22}z_2 \end{aligned} \tag{4.19}$$

As the matrix of the linear transformation is different in different orthonormal bases, only the basis (4.18) will be further assumed. Algebraically, representations of matrix groups when each matrix corresponds to itself, do not differ from other faithful representations and have no special mathematical name; physicists often call them "fundamental." The fundamental representation of SU(2) is irreducible: it is easily verified that no vector is carried by all transforms (4.19) into its own multiple; that is, there is no one-dimensional invariant subspace. From eq. (4.10), it follows that this representation is unitary. As was discussed in Chapter 2, the main observables of our quantum system are derived from the symmetry group SU(2) and are matrices of its Lie algebra. As we know, this Lie algebra consists of traceless second-order Hermitian matrices expressed as linear combinations of matrices $\tau_k = \frac{1}{2}\sigma_k$ ($k = 1, 2, 3$) with real coefficients (eq. (3.37)) and obeying commutation relations (eq. (3.76)). These basis matrices, with appropriate factors, are main observables of our system. Polynomial $\tau^2 = \tau_1^2 + \tau_2^2 + \tau_3^2$ is the Casimir operator and takes value $\frac{1}{2}\left(\frac{1}{2} + 1\right) = \frac{3}{4}$ for the fundamental representation.

Now construct the Hamiltonian. As was shown in Chapter 2, the Hamiltonian is an element of the universal enveloping algebra of the symmetry groups; in the case of "perfectly symmetrical" system, it commutes with the symmetry group, that is, proportional to the Casimir operator. *Electron* spin is an example of such perfectly symmetrical system. As the mass is proportional to the energy, we can identify the Hamiltonian of such a system with the operator of the weight. In nonrelativistic quantum mechanics, the energy is understood as just as a small addition to the "rest energy" due to the movement of the particles; but if space–time properties of the particle are not considered, this addition becomes insignificant and the energy must be regarded as the rest energy mc^2. This gives rise to the concept of mass operator identified (up to a factor) with the Hamiltonian. For the electron spin, mass operator should be regarded as a multiple of Casimir operator τ^2; therefore, all spin states of the electron are associated, according to the experience, with the same mass.

Now apply the same mathematical formalism to describe the "state of the nucleon." Two "distinguished" states of the system will be considered: the "proton state" and the "neutron state," as the analogs of electron states with spin projections $\left(S_z = \pm\frac{\hbar}{2}\right)$. To distinguish this new type of spin from the electron spin, we will call it the *isotopic spin*[34] or *isospin*. To avoid confusion, for the isospin case matrices, τ_k will be designated T_k. The observables T_1, T_2, T_3 of the isospin do not commute, and only one of them (let it be T_3) may have a definite value. The eigenvalues of T_3 are $\pm\frac{1}{2}$;

34 The term has nothing to do with the isotopes of the elements.

the corresponding spinors are $-e_1$ and e_2 (eq. (4.19)). It will be assumed that e_1 is the vector of the proton state, and e_2 is the vector of the neutron state of the nucleon (this agreement is conditional, since both vectors are equal). Then the charge of particles Q can be expressed in terms of T_3:

$$Q = T_3 + \frac{1}{2} \tag{4.20}$$

However, simple is the relation, such approach to the electric charge was unusual for the traditional quantum mechanics where the charge (along with the mass) was always considered a constant numerical characteristic of the particle rather than an *observable*, that is, a Hermitian operator acting on the state vectors. This point of view happened to be very fruitful.

In contrast to electron spin, isotopic spin is associated with mass splitting and, therefore, with *symmetry breaking* of the system. Therefore, the Hamiltonian (or the mass operator) is taken as

$$M = \alpha T^2 + \beta Q \tag{4.21}$$

where operator $\beta Q = \beta T_3 + \frac{\beta}{2}$ is added to the Casimir operator αT^2. Since T_3 belongs to the Lie algebra G of group SU(2), the polynomial M belongs, as follows from the general reasoning of Section 2.4, to its universal enveloping algebra $\widetilde{\mathrm{G}}$. Thus, the mass of the particle, like its charge, becomes an *observable* of the quantum theory. The neutron and the proton are represented by vectors of the nucleon state, which are eigenvectors of operator M, that is, considered as states with a certain mass. The second term in the mass formula (eq. (4.21)) is small as compared to the first due to small difference between the masses of the neutron and the proton; therefore, the second term in eq. (4.21) can be considered as a "perturbation" of the symmetric operator of the nucleon mass and explains the idea of "broken symmetry."

Along with the family of two nucleons considered by Heisenberg, there are other families of particles with very similar masses, that is, small differences between their masses compared with the masses themselves: three Σ particles Σ^-, Σ^0, and Σ^+ (charges –1, 0, +1), four Δ particles Δ^-, Δ^0, Δ^+, Δ^{++} (charges –1, 0, 1, 2), and so on. These families are called *isotopic multiplets* (a doublet of two particles, a triplet of three particles, a quadruplet of four particles, etc.) which are very important for particle classification. They are naturally described by representations of SU(2) of various dimensions like it was done in Section 4.1 for spin states of particles of any spin. Thus, three Σ particles are considered the states of a quantum system "Σ" with a three-dimensional state space C^3, where an irreducible representation of SU(2) group is defined, and so on. In all these spaces, the operators to define the Lie algebra of SU(2) are observables of the corresponding quantum system. Since the projection of isospin T_3 takes (integer or half-integer) values $-T, -T+1, \ldots, T-1, T$ which are, similar to the charges

of the particles of the multiplet, equidistant from each other, we can expect a relation between T_3 and Q. It turns out that

$$Q = T_3 + \frac{n}{2} \tag{4.22}$$

where n is a positive or negative integer number depending on the multiplet. The number of particles in the multiplet is $2T + 1$; the number T is called the *isospin* of all these particles. Expressing $T^2 = T_1^2 + T_2^2 + T_3^2$ in terms of T, obtain T(T+1), and, similar to angular momentum operators L_k, we have $L^2 = L(L + 1)$. Finally, mass splitting within the isotopic multiplet can be approximately described by a perturbing operator quadratic in Q; the obtained mass formula is

$$M = \alpha T(T + 1) + \beta + yQ + \delta Q^2 \tag{4.23}$$

where coefficients α, β, y, δ are multiplet dependent.

By analogy with the conventional quantum mechanics, mass splitting within isotopic multiplets can be regarded as a result of some "interaction." Without the "disturbing" term, all states would have the same masses, like electronic energy levels remain degenerate in a spherically symmetric field until the symmetry of the field is broken. When external magnetic field is applied, it starts interacting with the electron and virtually does not change while electron energy levels split into nondegenerate levels. The additional term in the mass formula can be considered as some interaction to break the symmetry of the "nucleon." The difference is that there are no "nucleons" with unbroken symmetry in nature. The electron in a perfectly Coulomb field is also an abstraction since even the proton as the nucleus is something more complex than a point charge. However, there is a sufficiently close approximation to the Coulomb symmetry to make the violations of this symmetry a perturbation of the *real* state of the system. Of course, in the case of "nucleons," the reality of exact SU(2) symmetry is out of the question. Further, there is no "interaction" with the *external* system: in fact, the "nucleon" interacts with itself similar to the electron which "receives weight" due to "self-action" even in the vacuum. Such generalization of the concepts of symmetric system state and interaction is very typical of modern quantum theory.

While usual systems have states described by infinite-dimensional Hilbert space of ψ functions and are interesting as far as their spatial–temporal behavior, in the case of isotopic multiplets, we are interested in the "internal degrees of freedom" of the particles, and the state space is a *finite-dimensional* Hilbert space. In other respects, it shares all main features of a quantum theory like Hilbert space of state vectors, representation of the symmetry group, construction of the observables from the Lie algebra of this group and its Hamiltonian from its universal enveloping algebra (i.e. in the form of polynomials of the operators of the Lie algebra using the Casimir operator of the group).

Temporal evolution of the system is not considered in this approach. Indeed, in ordinary quantum mechanics, a solution $\psi(x, y, z, t)$ of the Schrödinger equation is searched, and the task is reduced to finding eigenfunctions and eigenvalues of the Hamiltonian (since the temporal evolution for eigenfunctions ψ_n is given by the exponential factor $e^{-iE_n t/\hbar}$). The theory of isotopic multiplets does not contain the time, and the states of the multiplet with *certain masses* corresponding to elementary particles are defined by eigenvectors of the mass operator.

The situation is more complicated with the "superposition law." In the usual formulation, the principle states "if $\psi_1, \psi_2, \ldots$ are the state vectors of a quantum system, then all nonzero linear combinations $\lambda_1\psi_1 + \lambda_2\psi_2 + \cdots$ also are vectors to represent possible states of the system." Under the assumption that the state vectors form a Hilbert space, this simply means that the space is *linear*. However, there are cases when a Hilbert space is an appropriate tool to describe the system, but not all its vectors can be interpreted as representations of physically possible states. First, such a situation was met in quantum electrodynamics for systems with some (variable) number of electrons and positrons. The quantum theory formalism requires the states of such system to be defined by the vectors of the corresponding Hilbert space (the so-called "Fock space"). But if, for example, ψ_- is a state with some electron and ψ_+ is a state of some positron, the superposition $\alpha\psi_- + \beta\psi_+$ should be interpreted as a state of a particle which is an electron with probability $|\alpha|^2$ and a positron with probability $|\beta|^2$. Such state cannot be viewed real. Therefore, the applicability of the "superposition principle" should be limited: Hilbert spaces are considered a mathematical tool, but physical meaning is associated with the vectors from only some of its subspaces, for example, those with some certain charge. This is the essence of Wigner's "superselection rules" which is especially important in particle classification: if, for example, e_1 and e_2 image the proton and the neutron state of a nucleon, then for non-zero α, β linear combinations, $\alpha e_1 + \beta e_2$ do not represent real physical conditions of a nucleon (though they are necessary for its description, since the representation of a symmetry group is constructed in a *linear* space!) Only the vectors which are multiples of e_1 or e_2 represent physically real conditions of a nucleon. This view on the "superposition principle" is essential to understand further reasoning.

4.3 SU(3) group

In 1961, Gell-Mann (Calif, 1961) and Neeman (1961) independently suggested a classification of hadrons to combine isotopic multiplets in larger families. The idea will be outlined as a preparation to the following element classification. (A detailed discussion of the theory of unitary symmetry assuming only the fundamentals of quantum mechanics, see, for example, in Rumer and Fet, 1970.)

As mentioned above, mass splitting within isotopic multiplets is considered by analogy with energy levels splitting associated with a violation of the Hamiltonian symmetry, that is, when some interaction takes place. Such "symmetric" systems as "nucleon," "Σ," and so on, in their turn can be imagined as the results of violation of a higher symmetry of some hypothetical system due to its internal "interaction." Since average masses of isotopic multiplets are very far from each other, this interaction should be much stronger than the one to cause mass splitting within isotopic multiplets. It can be thought that before this "stronger" interaction, the system had higher symmetry, and therefore, a larger symmetry group than isotopic multiplets, and that symmetry violation is associated with a narrowing of this group to its subgroup SU(2). When the next "weaker" interaction is "turned on," the masses of isotopic multiplets finally split into the masses of individual real particles. The whole family of particles described by a "large" symmetry group is, therefore, combined by some "affinity": these particles are considered as *states of a single quantum system*. Particles from different isotopic multiplets should thus be considered not so much similar as those within the same isotopic multiplet, as splitting of the initial object into isotopic multiplets requires stronger interaction than the one needed to split the latter into individual particles. Thus, we obtain a "hierarchical" particle classification.

The group of unitary unimodular[35] matrices of the *third*-order SU(3) was suggested as a larger symmetry group. Its elements have the form $u = (u_{\sigma\tau})$, where $u_{\sigma\tau}$ are complex numbers and $\sum_{\rho=1}^{3} u^*_{\sigma\rho} u_{\tau\rho} = \delta_{\rho\tau}$, $(\sigma, \tau = 1, 2, 3)$, $\det|u_{\sigma\tau}| = 1$. Each such matrix defines a transform of a three-dimensional complex space C^3

$$\delta'_\sigma = \sum_{\tau=1}^{3} u_{\tau\rho} z_\tau, \quad (\sigma = 1, 2, 3), \tag{4.24}$$

the scalar product being preserved (see eq. (4.17)):

$$\langle z'|w'\rangle = \sum_{\sigma=1}^{3} z'^*_\sigma w'_\sigma = \sum_{\sigma=1}^{3} z^*_\sigma w_\sigma = \langle z|w\rangle \tag{4.25}$$

Equation (4.24) defines the three-dimensional unitary representation of SU(3) in the space C^3 which is irreducible: to prove it, it is enough to find such matrices in SU(3) that the corresponding operators of representation (4.24) translate some vector of C^3 (for example, $(z_1 = 1, z_2 = 0, z_3 = 0)$) into three linearly independent vectors of C^3 (which constitute a basis of this space). The reader is encouraged to do this simple exercise.

In contrast to the fundamental representation of SU(2) group, representation (4.24) is directly connected with the definition of the group and has no physical

35 With the unit determinant.

meaning for the reasons to be discussed later. Now consider Lie algebra of SU(3) group. To obtain unitary matrices u in the form e^{-iA}, *Hermitian* matrices of the third order should be taken as A matrices, and like it was the case of SU(2)group, *unimodular* matrices u are obtained from traceless matrices A. Consequently, the Lie algebra of SU(3) group consists of matrices

$$A = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{12}^* & a_{22} & a_{23} \\ a_{13}^* & a_{23}^* & a_{33} \end{bmatrix} \tag{4.26}$$

where a_{kk} are real and $\sum_{k=1}^{3} a_{kk} = 0$. There are eight independent real parameters to determine A: these are real and imaginary parts of elements a_{12}, a_{13}, a_{23} and two of the three real diagonal elements. Therefore, the dimension of the Lie algebra, and hence of SU(3) group, is eight. The basis of the Lie algebra is composed of any eight linearly independent traceless Hermitian matrices of order eight. The matrices will be obtained from nine Okubo matrices A_r^q (not all belonging to the Lie algebra) obeying the linear dependence $A_1^1 + A_2^2 + A_3^3 = 0$:

$$\begin{aligned}
A_1^1 &= \begin{bmatrix} 2/3 & 0 & 0 \\ 0 & -1/3 & 0 \\ 0 & 0 & -1/3 \end{bmatrix}, \quad A_1^2 = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad A_1^3 = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \\
A_2^1 &= \begin{bmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad A_2^2 = \begin{bmatrix} -1/3 & 0 & 0 \\ 0 & 2/3 & 0 \\ 0 & 0 & -1/3 \end{bmatrix}, \quad A_2^3 = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{bmatrix}, \\
A_3^1 &= \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix}, \quad A_3^2 = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}, \quad A_3^3 = \begin{bmatrix} -1/3 & 0 & 0 \\ 0 & -1/3 & 0 \\ 0 & 0 & 2/3 \end{bmatrix}.
\end{aligned} \tag{4.27}$$

All these matrices are traceless, but only three of them are Hermitian: A_1^1, A_2^2, A_3^3. Eight Gell-Mann matrices are expressed in terms of the Okubo matrices:

$$\begin{aligned}
\lambda_1 &= A_1^2 + A_2^1, \quad \lambda_2 = \frac{1}{i}(A_1^2 - A_2^1), \\
\lambda_4 &= A_1^3 + A_3^1, \quad \lambda_5 = \frac{1}{i}(A_1^3 - A_3^1), \\
\lambda_6 &= A_2^3 + A_3^2, \quad \lambda_7 = \frac{1}{i}(A_2^3 - A_3^2), \\
\lambda_3 &= A_1^1 - A_2^2, \quad \lambda_8 = -\frac{1}{\sqrt{3}} A_3^3.
\end{aligned} \tag{4.28}$$

(the numbering of the matrices and the coefficient $-\frac{1}{\sqrt{3}}$ at λ_8 are unessential and are used by tradition). As is easily verified, Gell-Mann matrices are traceless,

Hermitian, and linearly independent; thus, they form a basis of the Lie algebra of SU(3) group. And vice versa, Okubo matrices can be expressed from eq. (4.28) and $A_1^1 + A_2^2 + A_3^3 = 0$ as linear combinations of Gell-Mann matrices with complex coefficients:

$$\begin{aligned} A_1^2 &= \frac{1}{2}\lambda_1 + \frac{i}{2}\lambda_2, \quad A_2^1 = \frac{1}{2}\lambda_1 - \frac{i}{2}\lambda_2, \\ A_1^3 &= \frac{1}{2}\lambda_4 + \frac{i}{2}\lambda_5, \quad A_3^1 = \frac{1}{2}\lambda_4 - \frac{i}{2}\lambda_5, \\ A_2^3 &= \frac{1}{2}\lambda_6 + \frac{i}{2}\lambda_7, \quad A_3^2 = \frac{1}{2}\lambda_6 - \frac{i}{2}\lambda_7, \\ A_1^1 &= \frac{1}{2}\lambda_3 + \frac{\sqrt{3}}{2}\lambda_8, \quad A_2^2 = -\frac{1}{2}\lambda_3 + \frac{\sqrt{3}}{2}\lambda_8. \end{aligned} \tag{4.29}$$

Evidently, Okubo matrices belong to the complex envelope of the Lie algebra (see Section 3.3). As follows from eq. (4.29), commutation relations for λ_j matrices completely determine those for matrices A_σ^τ; conversely, if commutation relations for A_σ^τ are known, eq. (4.28) can be used to obtain commutation relations for λ_j. Commutation relations for Okubo matrices are even simpler, they are given by a single equation:

$$[A_\tau^\sigma, A_\mu^\lambda] = \delta_\mu^\sigma A_\tau^\lambda - \delta_\tau^\lambda A_\mu^\sigma \quad (\sigma, \tau, \lambda, \mu = 1, 2, 3) \tag{4.30}$$

where $\delta_\tau^\sigma = 1$ for $\sigma = \tau$ and $\delta_\tau^\sigma = 0$ for $\sigma \neq \tau$. The resulting commutation relations for λ_j can be easily derived.

According to Section 3.3, to construct a representation of SU(3) group in some space, operators T_{λ_j} with the same commutation relations as those for matrices λ_j are to be defined in this space. However, it is more convenient to proceed in a different way: first a correspondence is set up between matrices A_τ^σ and operators $T_{A_\tau^\sigma}$ with the same commutation relations (eq. (4.30)) as those for matrices A_τ^σ, and then $T_{A_\tau^\sigma}$ is used to express operators T_{λ_j} by the same linear combinations as eq. (4.28). Repeating the derivation of commutation relations for λ_j from those for A_τ^σ, the same commutation relations are obtained for T_{λ_j} as those for matrices λ_j and the needed representation is therefore constructed. For simplicity, we will write further A_τ^σ instead of operator $T_{A_\tau^\sigma}$. We will consider only unitary representations where operators A_σ^σ (σ=1,2,3) are Hermitian (along with λ_j).

In contrast to SU(2) group whose maximal system of the main commuting observables is a single matrix τ_k, SU(3) group has *two* such observables represented by any two matrices A_σ^σ. We take the observables A_1^1 and A_3^3. These matrices commute with each other but not with other A_τ^σ (except $A_2^2 = -A_1^1 - A_3^3$). In different representations, they correspond to commutation operators whose eigenvalues depend on the representation. Thus, in a three-dimensional representation (eq. (4.24)), these eigenvalues are $^2/_3$ and $^{-1}/_3$ for the vector (1,0,0); $^{-1}/_3$ and $^{-1}/_3$ for the vector (0,1,0); and $^{-1}/_3$

and $^2/_3$ for the vector (0,0,1), so that in this case, the values of the observables A_1^1, A_3^3 uniquely define basis vectors; however, as we will see, this representation (unlike the fundamental representation SU(2)) has no clear physical interpretation. In other representations, the eigenvalues of operators A_1^1, A_3^3 do not define basis vectors. The additional quantum number can be obtained from subgroup SU(3) constituted by matrices

$$\begin{bmatrix} u_{11} & u_{12} & 0 \\ u_{21} & u_{22} & 0 \\ 0 & 0 & 1 \end{bmatrix} \tag{4.31}$$

This subgroup can be defined as matrices u such that vector (0,0,1) is preserved under linear transformations (eq. (4.24)). Matrices (4.31) are evidently in a one-to-one correspondence with matrices SU(2) and are multiplied the same way as matrices SU(2); therefore, the subgroup (4.31) is *isomorphic* to SU(2) group; we denote it simply SU(2). So, there is a chain of groups:

$$SU(3) \supset SU(2) \tag{4.32}$$

Now construct a Lie subalgebra of SU(2) subgroup. As is seen from eq. (4.31), the generators of one-parameter subgroups SU(2) have zero elements in the third lines and in the third columns. Therefore, the basis of the subalgebra consists of matrices

$$\begin{aligned} T_1 &= \frac{1}{2}(A_2^1 + A_1^2) = \begin{bmatrix} 0 & ^1/_2 & 0 \\ ^1/_2 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \quad T_2 = \frac{1}{2i}(A_1^2 - A_2^1) = \begin{bmatrix} 0 & -^i/_2 & 0 \\ ^i/_2 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \\ T_3 &= A_1^1 + \frac{1}{2}A_3^3 = \begin{bmatrix} ^1/_2 & 0 & 0 \\ 0 & -^1/_2 & 0 \\ 0 & 0 & 0 \end{bmatrix} \end{aligned} \tag{4.33}$$

with the same commutation relations as those for τ_k (see eq. (1.12)). Matrices T_k define *isospin operators* in any representation SU(3), and Casimir operator $T^2 = T_1^1 + T_2^2 + T_3^3$ of SU(2) subgroup is constant on each irreducible space SU(2). In particular, after representation SU(3) is reduced to subgroup SU(2), we obtain irreducible subspaces SU(2) such that $T^2 = T(T+1)$ on each of them and which, therefore, have a definite value T of the isospin. By definition given in Section 2.2, quantum number is the value of the Casimir operator $T(T+1)$; but since it is determined by isospin value T, the latter is also called a quantum number. The dimension of this subspace is $2T+1$ and, as shown above, it has a basis composed of eigenvectors T_3 with eigenvalues $-T, -T+1, \ldots T-1, T$. All such bases together, by the definition of the reduction of a representation, constitute a basis of representation SU(3).[36] But since some of

36 Further, for the sake of brevity, we write "a basis of the representation" rather than "a basis of the representation space."

representations contain more than one irreducible subspace SU(2) of the same dimension, the vectors of this basis cannot be numbered by quantum numbers (T, T_3). If, however, two operators A_1^1 and $A_3^3$are taken instead of $T_3 = A_1^1 + \frac{1}{2}A_3^3$, then three quantum numbers (T, A_1^1, A_3^3) can be shown to define a one-to-one numbering of the basis of *any* representation of SU(3) group, that is different basis vectors correspond to different sets of these quantum numbers.

Unlike conventional quantum numbers such as (H, L, L_Z), the set (T, A_1^1, A_3^3) contains no eigenvalue of the energy operator (in our case, mass operator). This fact has two meanings. First, the states of the system described by some representation SU(3) can be classified by quantum numbers of the state which are associated with some physical meaning, while masses are not used. Second, if the mass operator M commutes with T^2, A_1^1, and A_3^3, then the eigenvectors of these three operators will be also eigenvectors of M and, therefore, the eigenvalues of M must be expressed in terms of these quantum numbers; if M *approximately* commutes with these three operators, then the states associated with quantum numbers can be considered as approximations to the states with definite masses.

We illustrate this approach on the example of the baryon octet, which is the first family of elementary particles described by SU(3) symmetry group.

4.4 Baryon octet and decuplet

In terms of the mass, elementary particles are divided into light particles, or leptons (electron, muon, various types of neutrinos, and their antiparticles), and heavy particles, or hadrons; also, there is the photon, which belongs to neither of these two categories. Besides the masses, these two groups of particles have more important differences associated with the nature of the interactions they participate in. Hadrons include particles with integer spin, or mesons, and particles with half-integer spin, or baryons. SU(3) group describes symmetry properties of hadrons and has no relation to the leptons and to the photon. Families of particles described by irreducible representations of this group consist either of baryons or mesons. It is natural to assume that particles from each family should have other common properties besides the common representation of the symmetry group. In the beginning, the theory of unitary symmetry considered mainly the eight most studied baryons with the same spin ½ and the same intrinsic parity +: the proton P and the neutron N with very close masses to form the isotopic doublet; two Ξ particles, Ξ^- and Ξ^0 (the superscripts indicate the charges measured in absolute values of the electron charge) which also have very close masses and considered an isotopic doublet; three Σ particles, Σ^-, Σ^0, and Σ^+ to constitute the isotopic triplet; and finally, Λ particle with zero charge and the mass differing from those of all other particles (such particle is associated with a one-dimensional representation of SU(2) group and is called an "isotopic singlet").

According to the above scheme of particle classification, these eight baryons is possibly described as states with definite mass values of some quantum system ("the octet") whose state space is the space of eight-dimensional irreducible representation of SU(3) group. Further, when reduced to the subgroup SU(2), this space should expand into the sum of irreducible subspaces of SU(2) subgroup whose dimensions correspond to the number of particles in the isotopic multiplets of the octet, that is 2, 2, 3, 1. Such representation of SU(3) group was in fact discovered, the charges and, in a sense, the masses of the particles were naturally described; from these eight particles came the allegorical name "Eightfold Way" given to SU(3) symmetry by its discoverers.[37]

Now the eight-dimensional irreducible representation of SU(3) will be described; Appendix B outlines the mathematical approach to obtain it (as well as the 10-dimensional representation that we will need below).

Consider an eight-dimensional complex space C^8 with coordinates $z_1, \ldots, z_8$ and the scalar product

$$\langle z|w\rangle = \sum_{\lambda=1}^{8} z_\lambda^* w_\lambda \tag{4.34}$$

Eight matrices of order eight can be defined to represent matrices A_τ^σ and to obey the same commutation relations (eq. (4.30)); let these matrices be denoted by the same letters. This will define a representation of basis matrices λ_j of Lie algebra with the same commutation relations, and, therefore, a representation of SU(3) group in space C^8 which turns out to be irreducible. Since the matrices representing λ_j turn out to be Hermitian, the constructed representation is unitary. The above method of using Lie algebras provides only local (defined only in the vicinity of the identity) representations of the group; however, for SU(3) group, the representation of the Lie algebra can be proved to correspond to a global representation (uniquely defined on the whole group). The representation matrices would be hardly understandable without preceding derivation, so we will describe only the properties of this representation. Each matrix of representation A_τ^σ defines the operator in C^8:

$$z'_\lambda = \sum_{\mu=1}^{8} (A_\tau^\sigma)_{\lambda\mu} z_\mu \quad (\lambda = 1, \ldots, 8), \tag{4.35}$$

where $\sigma, \tau = 1, 2, 3$ designate the number of the operator corresponding to the number of the matrix (eq. (4.27)); if the orthonormal basis in C^8 is properly chosen, all basis vectors are eigenvectors of the commuting operators A_1^1, A_3^3 together with $T_3 = A_1^1 + \frac{1}{2}A_3^3$. Table 4.1 shows the corresponding eigenvalues for some numeration of the basis. Further, it turns out that the representation is reduced to subgroup SU(2), space C^8 is decomposed into the orthogonal sum of the following irreducible subspaces of SU(2):

37 This name is borrowed from the Indian philosophy where it means "the right way" in quite a different sense.

one three-dimensional space, two two-dimensional spaces, and one one-dimensional space. For the chosen numeration of basis vectors, one of the two-dimensional subspaces is generated by vectors e_1, e_2, the three-dimensional space is generated by vectors e_3, e_4, e_5, one-dimensional space by vector e_6, and the second two-dimensional by vectors e_7, e_8 (the actual reason for such numeration will be explained below). The decomposition is as follows:

$$C^8 = C^2 \oplus C^3 \oplus C^1 \oplus C^{2'} \tag{4.36}$$

Casimir operator $T^2 = T_1^2 + T_2^2 + T_3^2$ of the subgroup SU(2) has on these subspaces constant values $T(T+1) = \frac{3}{4}, 2, 0, \frac{3}{4}$, respectively; therefore, the values of the isospin T on subspaces are $\frac{1}{2}, 1, 0, \frac{1}{2}$. All these data are presented in Table 4.1.

Table 4.1: Eigenvalues and the values of Casimir operator on the irreducable subspaces.

Particle	Mass, MeV	A_1^1	A_3^3	T
Ξ^-	1320.8	−1	1	1/2
Ξ^0	1314.3	0	1	1/2
Σ^-	1197.1	−1	0	1
Σ^0	1192.4	0	0	1
Σ^+	1189.4	1	0	1
Λ	1115.4	0	0	0
N	939.5	0	−1	1/2
P	938.3	1	−1	1/2

Now quantum numbers (A_1^1, A_3^3, T) in the constructed eight-dimensional representation receive a physical interpretation. To begin with, the decomposition in the SU(2) subgroup corresponds exactly to isotopic multiplets of the family of eight baryons: two two-dimensional subspaces correspond to doublets Ξ and N, the three-dimensional subspace corresponds to triplet Σ, one-dimensional subspace corresponds to singlet Λ. Quantum number T defines therefore the number of particles $2T + 1$ in the isotopic multiplet containing the given particle. The isospin of a particle is its "collective" property: to find it experimentally, it is not enough to know this particle, rather we have to know the number of particles with close masses which form together with it the isotopic multiplet. Quantum number T distinguishes between multiplets only with different number of particles while quantum number A_3^3 is used to distinguish between multiplets with the same number of particles. As is seen from eq. (4.30), matrix A_3^3 commutes with the isospin matrices (eq. (4.33)), and therefore with all matrices of subgroup SU(2). Thus, A_3^3 (along with T^2) is a Casimir operator of this subgroup. The values of A_3^3 on C^2 and $C^{2\prime}$ (1 and –1, respectively) (Table 4.1) distinguish these subspaces. Later we will discuss physical interpretation of A_3^3 in more detail.

Physical meaning of quantum number A_1^1 is immediately seen when comparing Table 4.1. with the charges of eight baryons: for e_1, e_2, e_3, e_4, e_5, e_6, e_7, e_8 eigenvalues of A_1^1 are, respectively, the charges of particles Ξ^-, Ξ^0, Σ^-, Σ^0, Σ^+, Λ, N, P. Thereby, operator A_1^1 in the eight-dimensional representation can be identified with the *operator of charge Q* which, therefore, has the meaning of the *main observable of* SU(3) *group*. The values of A_1^1 belonging to the basis vectors e_1, ..., e_8 explain the chosen numeration of the basis: it corresponds to the eight baryons arranged in the in descending order of the weights. Now the meaning of quantum number A_3^3 becomes clear: as can be seen from Table 4.1, $-A_3^3$ is the double average of the particle charges contained in the isotopic multiplet. The observable $Y = -A_3^3$ is called a *hypercharge* of the particle; similar to the isospin, it is a "collective" property of a particle. Even before the SU(3) theory was developed, Y had been known to take integer values for all particles; Table 4.1 corresponds to this experimental fact.

As Table 4.1 shows, state vectors of the octet to represent eight baryons with spin ½ can be given by the eigenvalues of Casimir operators T^2, Y of SU(3) subgroup, and the eigenvalue of operator Q of the Lie algebra of SU(3) group. Table 4.2 shows the relation between the particles from the baryon octet with the quantum numbers of SU(3) group. The masses of the particles are not yet described by the theory; this will be done later using the "mass formula." Thus, it is clear that quantum numbers T, Y, Q have a group origin: they relate to the chain of groups (eq. (4.32)). Since the baryon octet is associated with an eight-dimensional irreducible representation of SU(3) group, and operators T^2, Q, Y could be interpreted as operators of the isospin, the charge, and the hypercharge, respectively, it can be suggested that other irreducible representations SU(3) also describe some natural families of particles, and operators T^2, Q, Y have the same physical meaning also in other representations. The assumption will be shown true for the baryon decuplet.

Table 4.2: Relation between the particles from the baryon octet with the quantum numbers of SU(3) group

Particle	Q	Y	T	T_3
Ξ^-	−1	−1	1/2	−1/2
Ξ^0	0	−1	1/2	1/2
Σ^-	−1	0	1	−1
Σ^0	0	0	1	0
Σ^+	1	0	1	1
Λ	0	0	0	0
N	0	1	1/2	−1/2
P	1	1	1/2	1/2

Consider a 10-dimensional irreducible representation of SU(3). As is shown in Appendix B, it can be constructed by the same general method as the eight-dimensional

representation. Matrices A_τ^σ are associated with the 10$^{\text{th}}$-order matrices to define linear operators in the 10-dimensional complex space C^{10} with commutation relations (eq. (4.30)). This defines an irreducible 10-dimensional representation of SU(3)group. It is also unitary, as matrices of the Lie algebra correspond to *Hermitian* matrices. When reducing the representation to the subgroup SU(2), C^{10} is expanded into one four-dimensional, one three-dimensional, one two-dimensional, and one one-dimensional irreducible subspaces of SU(2):

$$C^{10} = C^1 \oplus C^2 \oplus C^3 \oplus C^4 \tag{4.37}$$

As basis vectors, common eigenvectors e_k of operators A_1^1, A_3^3 are chosen. They are numerated the way that e_1 generates subspace C^1; e_2, e_3 generate subspace C^2; e_4, e_5, e_6 generate subspace C^3; e_7, e_8, e_9, e_{10} generate subspace C^4. Table 4.3 shows the corresponding eigenvalues A_1^1, A_3^3 and the values of isospin operators T_3 and T^2 (T is presented instead of $T(T+1)$). Casimir operators T^2 and A_3^3 of subgroup SU(2), like in the case of the eight-dimensional representation, distinguish between irreducible subspaces of SU(2), but only one of them is needed since their eigenvalues are dependent *in the 10-dimensional representation*: $A_3^3 = 2(1 - T)$. Three quantum numbers (T, A_3^3, A_1^1) (actually, only the pair (T, A_1^1) or (A_1^1, A_3^3)) completely defines a basis vector.

Table 4.3: Eigenvalues of operators A_1^1 and A_3^3

Particle	Mass, MeV	A_1^1	A_3^3	T
Ω^-	1679	−1	2	0
Ξ_δ^-	1535	−1	1	1/2
Ξ_δ^0	1535	0	1	1/2
Σ_δ^-	1385	−1	0	1
Σ_δ^0	1385	0	0	1
Σ_δ^+	1385	1	0	1
Δ_δ^-	1238	−1	−1	3/2
Δ_δ^0	1238	0	−1	3/2
Δ_δ^+	1238	1	−1	3/2
Δ_δ^{++}	1238	2	−1	3/2

Physically, 10-dimensional representation is interpreted by comparing it with known particles. When SU(3) symmetry was proposed in 1961, *nine* baryons with the same spin $\frac{3}{2}$ and the same parity 4 were known to constitute isotopic multiplets: doublet Ξ_δ of particles $\Xi_\delta^-, \Xi_\delta^0$, triplet Σ_δ of particles $\Sigma_\delta^-, \Sigma_\delta^0, \Sigma_\delta^+$, and quadruplet Δ_δ of particles $\Delta_\delta^-, \Delta_\delta^0, \Delta_\delta^+, \Delta_\delta^{++}$ (upper indices show the charge). When comparing the multiplets with Table 4.3, we can see that they correspond exactly to the subspaces C^2, C^3, C^4, and vectors $e_2, e_3, e_4, e_5, e_6, e_7, e_8, e_9, e_{10}$ should, according to the charge $Q = A_1^1$, represent

particles $\Xi_\delta^-, \Xi_\delta^0, \Sigma_\delta^-, \Sigma_\delta^0, \Sigma_\delta^+, \Delta_\delta^-, \Delta_\delta^0, \Delta_\delta^+, \Delta_\delta^{++}$, respectively. Thus, Q is again interpreted as the operator of charge. The eigenvalues $Y = -A_3^3$ are again double average (integer) charges of the particles of the isotopic multiplet which confirms the interpretation of Y as a hypercharge operator.

However, in 1961, there remained an empty space in Table 4.3; vector e_1 did not correspond to any known particle. *Nine* baryons could not be described by an irreducible representation of SU(3) group which has no nine-dimensional irreducible representation; therefore, a correct description of isotopic multiplets and charges would require a *10-dimensional representation*. This way a lacking tenth particle could be predicted: Table 4.3 shows that it should be a singlet with charge –1. Since all other particles in Table 4.3 had the usual spin 3/2, it could be predicted that the lacking particle should be of the same spin. Moreover, its mass also could be predicted: as follows from the mass formula (§5), the masses of the particles of the decuplet are equidistant, that is, are spaced with the same value as is confirmed by experimentally measured masses; the mass of the tenth particle could be found from the differences between the masses of the rest nine particles.

In 1964, there was discovered a particle Ω^- which had all these properties. It was a triumph of theoretical physics like the prediction of lacking elements by Mendeleev or of a lacking planet by Adams and Le Verrier. Table 4.4 shows the relation between the baryon decouplet and the 10-dimensional representation of SU(3).

Table 4.4: Relation between the baryon decouplet and the 10-dimensional representation of SU(3).

Particle	Q	Y	T	T_3
Ω^-	−1	−2	0	0
Ξ_δ^-	−1	−1	1/2	−1/2
Ξ_δ^0	0	−1	1/2	1/2
Σ_δ^-	−1	0	1	−1
Σ_δ^0	0	0	1	0
Σ_δ^+	1	0	1	1
Δ_δ^-	−1	+ 1	3/2	−3/2
Δ_δ^0	0	+ 1	3/2	−1/2
Δ_δ^+	1	+ 1	3/2	1/2
Δ_δ^{++}	2	+ 1	3/2	3/2

Irreducible representations of SU(3) have dimensions $N(p,q) = \frac{1}{2}(p+1)(q+1)(p+q+2)$, where p, q are non-negative integers[38]; hence $N = 1, 3, 6, 8, 10, 21, 24, 27, 28, 35, 36, 42, 45, 48, 55, \ldots$ The eigenvalues of operators corresponding in these

38 A detailed discussion of the representations of SU(3) group see in Rumer and Fet (1970, ch. 5).

representations to matrices $Q = A_1^1$ and $Y = -A_3^3$ of the Lie algebra depend on the representation and should, as is seen from the examples of the octet and the decuplet, be interpreted as the values of the charge and the supercharge. Experimentally (though not theoretically), values of Q and Y are known to be always *integer*. Therefore, we obtain an empirical method to "discard" representations: only those with integer values of operators Q, Y are allowable. Then the dimensions of allowable representations $N(p, q)$ require the condition of p-q being a multiple of 3,[39] that is, $N = 1, 8, 10, 27, 28, 35, 55, \ldots$ Currently, we know many octets and decuplets consisting of hadrons (or baryons, or mesons); besides, there are "SU(3)-singlets", that is, hadrons corresponding to the one-dimensional representation of SU(3) and thus having no "similar" particles in the sense of this symmetry group. Other dimensions of "allowable" representations, beginning with 27, apparently do not describe any family of known particles; supposedly, the particles of higher representations are unstable and therefore cannot be observed.

4.5 Mass formula in the SU(3) symmetry

In ordinary quantum mechanics where symmetry group is a group of space–time transformations or some of its subgroup, the energy operator is a polynomial of the operators of the Lie algebra of the symmetry group. Thus, the Hamiltonian is expressed in terms of the momentum, the coordinate, the momentum projections, and the spin. But now, we have a symmetry group not related to the space–time behavior of the particles. The "interaction" to split the "octet" or the "decuplet" into "isotopic multiplets" and then into particles relates to the so-called *internal degrees of freedom* of a quantum system which are similar to the spin, as is exemplified by the isotope mass splitting. In a sense, what is discussed here are energy effects associated with the interaction of dynamic "spin" variables. Therefore, the set of observables originating from SU(3) group is sometimes called a "unitary spin." The formal method to construct the Hamiltonian remains the same: mass operator is constructed as a polynomial of the observables of the quantum theory, that is, in this case, the operators of the Lie algebra of SU(3) group. This operator acts in the representation space of SU(3) group which defines the quantum system, for example, in the eight-dimensional space of the octet or in the 10-dimensional space of the decuplet.

Elementary particles are considered as states of the system with certain masses, that is, as pure states of the mass operator, while particle masses are considered as corresponding eigenvalues. Thus, particles with $\Xi^-, \ldots, P$ should be represented by eigenvectors of the mass operator from C^8. But we have already found in C^8 eigenvectors of operators T^2, Y, Q having definite values of isospin, charge, and hypercharge

39 See Rumer and Fet (1970, ch. 11).

and uniquely described by these values (as always, up to a factor). If certain values of these observables correspond to actually existing particles, basis vectors should image the same octet states as the eigenvectors of the mass operator. In other words, the mass operator should commute with T^2, Y, Q and its eigenvalues should be expressed in terms of quantum numbers used above to specify basis vectors. In fact, if the values T, Y, Q are given, then their common eigenvector and, thereby, the mass M is also known.

The actual situation is somewhat more complicated: real particles have, of course, definite masses and charges, but their "isotopic relationship" is not so definite. Roughly speaking, a particle with a given charge seems to be mainly associated with some isotopic multiplet (e.g. Σ^0 with a triplet, Λ with a singlet); but to some extent, it is also associated with some other isotopic multiplet containing a particle of the same charge (e.g. Λ with a triplet, Σ^0 with a singlet). Mathematical expression of this so-called "mixing" of the particles is that state vectors with definite masses only approximately coincide with the vectors defined by quantum numbers T, Y, Q.

But then the expression of mass operator M can contain also other observables of SU(3) group. A good description of masses is obtained by suggesting that besides SU(2) subgroup (eq. (4.31)) consisting of the matrices to transform only z_1, z_2 but not z_3 there is another subgroup of the same type whose matrices do not change z_1. Designate this group $SU(2)'$ and write down, along with the main chain of groups (eq. (4.32)), also another chain which plays a role in the symmetry of the octet particles:

$$SU(3) \supset SU(2)' \tag{4.38}$$

The new isospin associated with this subgroup is called "U-spin," in contrast to "T-spin," that is, ordinary isospin described above by chain (eq. (4.32)). A detailed discussion of this subject is seen in Rumer and Fet (1970, ch. 9, 14, 15, 18).

Since the splitting of octet masses is clearly "hierarchical," that is, associated with great differences between the masses of isotopic multiplets and small differences inside them, mass operator M is naturally supposed to have a "step-like" nature like the classical Hamiltonian (eq. (1.81)):

$$M = M_0 + M_1 + M_2, \tag{4.39}$$

where M_0 is the Casimir operator of SU(3) group, M_1 is the Casimir operator of SU(2) subgroup, and M_2 is the operator constructed from the observables of SU(3) group but not of SU(2) subgroup. Equation (4.39) describes therefore a consistent symmetry breaking to split octet (or decuplet) masses.

Gell-Mann (1962) and Okubo (1962) derived the mass formula of such structure.[40] M_0 is constant in this formula for the given representation of SU(3). The "first perturbation"

40 Here only the final result is presented. See Rumer and Fet (1970, ch. 17).

$$M_1 = \alpha + \beta Y + y\left[T(T+1) - \frac{1}{4}Y^2\right] \tag{4.40}$$

where α, β, y the are constants depending on the representation (and not derived from the theory), Y and T^2 are the Casimir operators of SU(2) subgroup, and operator $T^2 = T_1^2 + T_2^2 + T_3^2$ is replaced by its value $T(T+1)$ on the isotopic multiplet. Perturbation M_1 *breaks* SU(3) symmetry but preserves SU(2) symmetry. Finally, the "second perturbation"

$$M_2 = \alpha' + \beta' Q + y'\left[U(U+1) - \frac{1}{4}Q^2\right] \tag{4.41}$$

has the same form but is related to the subgroup of *U spin* because it contains Casimir operators Q and $U^2 = U_1^2 + U_2^2 + U_3^2$ of this subgroup. With respect to the main chain of symmetry (eq. (4.32)), the term M_2 represents SU(2)-*symmetry breaking*.

The term (4.40) is of the most importance. From eq. (4.40) obtain for the octet "average masses" of isotopic multiplets: substituting values T, Y from Table 4.2 and designating m_0 the value of operator M_0, we have

$$\begin{aligned} m_\Xi &= m_0 + \alpha - \beta + \frac{1}{2}y, \\ m_\Sigma &= m_0 + \alpha + 2y, \\ m_\Lambda &= m_0 + \alpha, \\ m_N &= m_0 + \alpha + \beta + \frac{1}{2}y. \end{aligned} \tag{4.42}$$

The question arises how the validity of the mass formula can be verified if the constants (m_0, α, β, y) are unknown. Since all expressions (eq. (4.42)) contain the term $m_0 + \alpha$, there are *three* unknown constants $m_0 + \alpha, \beta, y$ and *four* equations. Excluding these constants, easily obtain the relation between the masses of isotopic multiplets:

$$m_\Xi + m_N = \frac{1}{2}(3m_\Lambda + m_\Sigma) \tag{4.43}$$

Though the masses cannot be found theoretically, eq. (4.43) can be verified by substituting experimental data (in MeV):

$$m_\Xi = 1318, \quad m_\Sigma = 1192, \quad m_\Lambda = 1115, \quad m_N = 939$$

Expressing m_Ξ in terms of other masses, obtain from eq. (4.43) that $m_\Xi = 1330$ which is <1% different from the experimental value.

Gell-Mann–Okubo mass formula is true for any multiplet of SU(3) group, for example, for the baryon decuplet discussed in Section 4.4. Considering only average masses of isotopic multiplets, that is, the term M_1, we find from Table 4.4 that the number $\delta = T - \frac{1}{2}Y$ is the same (=1) for all isotopic multiplets (this is a special property of the 10-dimensional representation of SU(3), but not of other representations). Expressing M in terms of Y and δ, obtain:

$$T(T+1)-\frac{1}{4}Y^2=\left(\frac{1}{2}Y+\delta\right)\left(\frac{1}{2}Y+\delta+1\right)-\frac{1}{4}Y^2=\frac{1}{2}Y(2\delta+1)+\delta(\delta+1),$$
$$M_1=\left(\beta+\delta+\frac{1}{2}\right)Y+(\alpha+\delta^2+\delta)=\left(\beta+\frac{3}{2}\right)Y+(\alpha+2)$$

Evidently, when Y increases by unity, the mass grows by the same value. But Table 4.4 shows that $Y=-A_3^3$ increases by unity when the number of the particles of the isotopic multiplet increases; thus, the masses of the singlet, the doublet, the triplet, and the quadruplet to constitute the decuplet should form an equidistant sequence $m_{\Delta_\delta}-m_{\Sigma_\delta}=m_{\Sigma_\delta}-m_{\Xi_\delta}=m_{\Xi_\delta}-m_\Omega$. The experimental masses known in 1961 were

$$m_{\Xi_\delta}=1532,\quad m_{\Sigma_\delta}=1385,\quad m_{\Delta_\delta}=1238,$$

so that the first two differences were –147. Hence the mass of the lacking particles can be predicted as $m_\Omega=m_{\Xi_\delta}+147=1679$ which coincides with the experimental value of Ω^- particle.

4.6 SU(6) group

In 1964, a wider group of symmetry was suggested to contain SU(3) as a subgroup. It was SU(6) group of sixth-order unitary matrices with determinant 1 (Gürsey and Radicati (1964), Pais (1964)). We discuss here only the facts needed to describe the Mendeleev homologous series.

SU(6) group is intended to describe both the "unitary spin" and the "conventional spin." Therefore, it should contain subgroups isomorphic to SU(3) and SU(2). The first of them (designated simply SU(3)) consists of matrices

$$U_F=\left[\begin{array}{c|c}u(3) & 0\\ \hline 0 & u(3)\end{array}\right] \tag{4.44}$$

where $u(3)$ is a matrix of SU(3) group. Matrices U_F are multiplied the same way as the corresponding unitary matrices of the third order $u(3)$; therefore, eq. (4.44) actually defines a subgroup isomorphic to SU(3). The second subgroup (designated simply SU(2)) consists of matrices

$$U_J=\left[\begin{array}{c|c}u_{11}e(3) & u_{12}e(3)\\ \hline u_{21}e(3) & u_{22}e(3)\end{array}\right] \tag{4.45}$$

where $e(3)$ is the identity matrix of the third order, and $(u_{\sigma\tau})(\sigma,\tau=1,2)$ form matrix u of SU(2) group. It is easily verified that matrices U_J are multiplied the same way as the corresponding second-order matrices u, that is, from $u_3=u_1u_2$, it follows that $U_{3J}=U_{1J}U_{2J}$, and hence the subgroup U_J is isomorphic to SU(2).

Lie algebra of SU(6) includes, on one hand, operators of the Lie algebra of SU(3) subgroup such as A_1^1, A_3^3, and so on, represented by sixth-order matrices

$$\left[\begin{array}{c|c} A(3) & 0 \\ \hline 0 & A(3) \end{array}\right], \tag{4.46}$$

where $A(3)$ is the third-order traceless Hermitian matrix such as A_1^1, A_3^3, and so on, and, on the other hand, operators of SU(2) subgroup such as s_k represented by sixth-order matrices

$$\left[\begin{array}{c|c} a_{11}e(3) & a_{12}e(3) \\ \hline a_{21}e(3) & a_{22}e(3) \end{array}\right] \tag{4.47}$$

where $(a_{\sigma\tau})$ is the traceless second-order Hermitian matrix, for example, τ_k. In any representation of SU(6), the operators to represent matrices (4.46) play the role of the operators of the unitary spin (isospin, charge, and hypercharge), while the operators to represent matrices (4.47) play the role of the operators of the ordinary spin. Evidently, subgroups SU(3) and SU(2) commute; therefore, the observables of the unitary spin (eq. (4.47)) commute with those of the ordinary spin (eq. (4.69)). Thereby, $T_k, Y, Q, \ldots$ are Casimir operators of subgroup SU(2), and s_1, s_2, s_3 are Casimir operators of subgroup SU(3). Together with the subgroup of isotopic spin $SU(2)_T$ which is part of SU(3) (and which should not be confused with the above subgroup of ordinary spin!), we have a chain of groups to define SU(3)-symmetry of elementary particles:

$$SU(6) \supset SU(3) \supset SU(2)_T \tag{4.48}$$

Not all dimensions have irreducible representations of SU(6). If the charge and hypercharge eigenvalues are requested to be integers, then only dimensions 1, 20, 35, 56, 70, 189, 405,… are allowed. The most important are 56-plet barions and 35-plet mesons filled with already known particles. We have considered only the first of them (see Rumer and Fet (1970, ch.13) for detailed discussion).

It can be shown that there is a 56-dimensional irreducible unitary representation of SU(6) which decomposes into the following irreducible representations of SU(3) subgroup: four 10-dimensional and two eight-dimensional representations. The value of the Casimir operator s_2 is $\frac{3}{2}\left(\frac{3}{2}+1\right)$ on the 10-dimensional subspaces, and $-\frac{1}{2}\left(\frac{1}{2}+1\right)$ on the eight-dimensional subspaces. The values of the Casimir operator s_3 are $^{-3}/_2$, $^{-1}/_2$, $^{1}/_2$, $^{3}/_2$ on the 10-dimensional subspaces, and $^{-1}/_2$, $^{1}/_2$ on the eight-dimensional subspaces. Designating them by corresponding indices, obtain the decomposition

$$C^{56} = C^{10}_{-3/2} \oplus C^{10}_{-1/2} \oplus C^{10}_{1/2} \oplus C^{10}_{3/2} \oplus C^{8}_{-1/2} \oplus C^{8}_{1/2} \tag{4.49}$$

The representations of subgroup SU(3) on the irreducible subspaces of C^{10} and C^8 are equivalent to those for baryon decuplet and baryon octet, respectively. Therefore, in all these subspaces, eigenvectors for the observables T^2, Y, Q can be chosen, as

it was done above. The resulting orthonormal basis of C^{56} is interpreted as follows: each eigenvector with given values T, Y, Q, s, s_3 represents the state of the 56-plet corresponding to the particle of the decouplet $(\Omega, \Xi_\delta, \Sigma_\delta, \Delta_\delta)$ or the octet $(\Xi, \Sigma, \Lambda, N)$ with the same values T, Y, Q and the projection of the *ordinary* spin s_3. For example, the vector with $T = 1/2, Y = 1, Q = 1, s = 1/2, s_3 = -1/2$ represents the proton with spin $-1/2$.

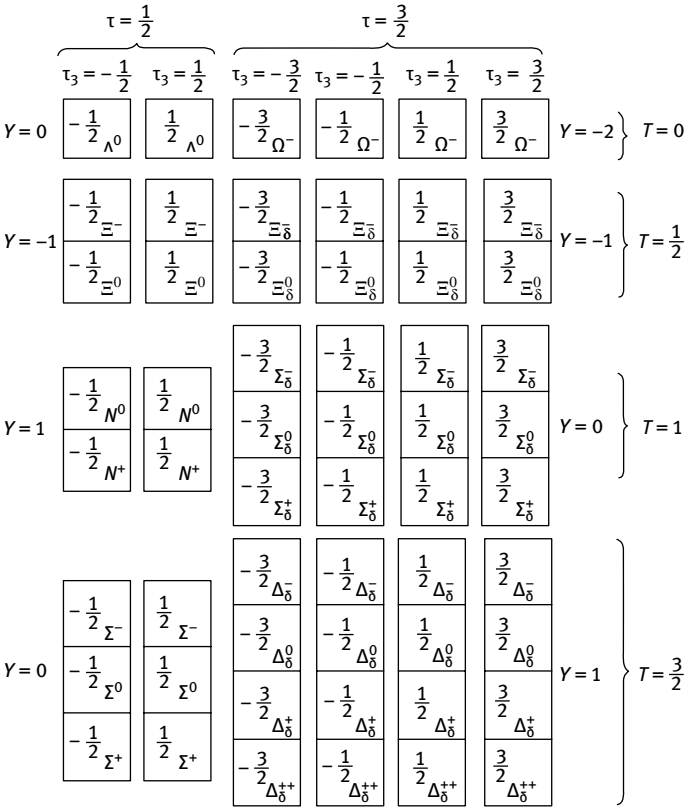
Thus, physical interpretation of the "states of the 56-plet" combine the meanings of the unitary and the ordinary spins: each state is not only a certain elementary particle as far as its mass, charge, and so on, but also its spin state. This viewpoint is natural to the group classification of particles, though differs from the approach of the experimental physics. In fact, the very concept of the "elementary particle" depends on the symmetry group underlying its description. As shown by Wigner, the common use of the term is associated with the Poincare group. If a family of particles is described by some irreducible representation of group G and is classified according to the chain of subgroups of G to characterize this symmetry, then basis vectors are naturally assumed to be associated with certain quantum numbers of group G corresponding to the "elementary particles" of this group. The eigenvalues of the mass operator may happen to be degenerate, so that different (in the above sense) particles have the same masses. For example, when describing the ordinary electron spin *by* SU(2) *group*, the electron states with $s_3 = -1$ and $s_3 = 1/2$ are to be considered *different* particles of the same mass. Note once again that the concept of "elementary" particle does not exist independently on its theoretical description, and since such description is determined by the symmetry group, the resulting ambiguity of the term should not be a surprise. Group classification of particles should base on the concepts associated with the chosen symmetry group rather than tradition.

Table 4.5 shows the classification of the 56-plet baryons in SU(6) symmetry. The values of the charge Q and spin projection s_3 are indicated by the right and left superscripts of the particle symbol, respectively. The proton P is designated N^+.

Vertical columns of Table 4.5 image the multiplets of the largest symmetry subgroup SU(3) (see eq. (4.48)), that is, two octets and four decuplets. Each vector of the basis is assumed, as in the case of SU(3) symmetry, to correspond to the individual particle.

When expanded in terms of the next subgroup SU(2) of the chain (4.48), each multiplet SU(3) splits into multiplets of $SU(2)_T$ subgroup imaged by the rectangles of Table 4.5. Each of these "small" multiplets is characterized by values T^2, Y of the Casimir operators of this subgroup (the eigenvalues $T(T+1)$ of the first of them are replaced by corresponding values T having no direct algebraic sense). Finally, individual particles are distinguished by sets (s, s_3, T, Y, Q) of quantum numbers of SU(6) group to define the "address" of the particle in Table 4.5. The classification presented in Table 4.5 corresponds to physical properties of the particles. In fact, the multiplets of the smallest subgroup $SU(2)_T$ are isotopic multiplets of closely similar particles. Multiplets of the larger subgroup contain particles which are more distantly related by SU(3)-symmetry. Compared to SU(3) group, SU(6) symmetry gives an additional quantum number s to describe the spin of octet particles and the spin $3/2$ of the decuplet particles.

Table 4.5: Classification of the 56-plet baryons in SU(6) symmetry.



SU(6) classification corresponds to the mass formula (Beg and Singh, 1964)[41] which we do not discuss here. As already mentioned, the eigenvalues of the mass should be degenerate due to the (ordinary) spin. Similarly, the 35-plet of mesons is classified; there is also a number of particles apparently belonging to the 20-plet and the 70-plet.

If, according to the group theoretical viewpoint, the 56-plet is assumed to describe 56 "elementary particles of SU(6) group," then there are not only "large" and "small" multiplets but also "mostly close" particles which differ only by the spin projection s_3 and standing in the same line of Table 4.5, for example, ${}^{-\frac{1}{2}}\Xi^0$, ${}^{\frac{1}{2}}\Xi^0$ or ${}^{-\frac{3}{2}}\Omega^-$, ${}^{-\frac{1}{2}}\Omega^-$, ${}^{\frac{1}{2}}\Omega^-$, ${}^{\frac{3}{2}}\Omega^-$. There is a method to specify these closest analogs: the Lie algebra of SU(6) group contains operators $s_+ = s_1 + is_2$, $s_- = s_1 - is_2$ transforming these similar particles into each other, and these operators commute with the operators of the unitary spin which act inside "large" multiplets (see Fet, 1975, p. 326). The same

41 See also Rumer and Fet (1970, ch. 17).

is true for the meson 35-plet. Further general ideas of group classification will be discussed to specify series of similar particles. It will be shown that this principle applied to the classification of chemical elements provides a natural algebraic description of Mendeleev homologous series such as alkali metals, alkaline earth metals, and so on, and explains Seaborg's analogy between lanthanides and actinides.

4.7 Classification principles in a quantum theory

The examples discussed in Chapters 1, 2, and 4 illustrate the general concept of classifying the states of quantum systems. The concept is equally true for classical systems such as atoms, molecules, or individual elementary particles, and for generalized systems such as "isotopic multiplet," "octet," "decuplet," and so on. Stationary states, that is, those with a definite energy, are always most interesting. In classical problems of quantum mechanics, the energy is viewed as a small addition to the rest mass and stationary states are certain excited states of atoms, molecules, and so on, such as, $s-$, $p-$, $d-$, and $f-$ states of the hydrogen atom. In the theory of hadron multiplets, where the energy is the rest mass, stationary states are the states with certain values of the mass multiplet corresponding to multiplet particles, for example, Ξ^-, Ξ^0, Σ^-, and so on. Classification principles are the same in all cases. First, we will discuss the classification of states in general, and then, pursuing our goals, classification of particles.

Any change in the state of a quantum system is called a *quantum transition*. Simplest transitions have geometric or kinematic nature when the system changes its position in space as a whole or starts a constant motion. These transitions are idealized descriptions of some interaction processes such as control of the electron or ion beam with an external electromagnetic field. Since the field in this interaction can be considered constant, it is not a part of the quantum system; therefore, "active" interpreting of such transitions is formal and does not take into account other systems to cause these transitions.

In a more common sense, the term "interaction" implies reactions between the particles. A full description of the reaction includes *all* involved particles, so that the initial and the final set of the (same or different) particles with the parameters of their motion are considered the states of the same system. But in some cases, it is possible to focus on some particles and to neglect others by excluding them from the system. If, for example, we consider baryons and mesons and neglect leptons, the reaction $N \to Pe^-\nu$ of a neutron decay into a proton, an electron, and a neutrino, can be considered a transition of the system $N \to P$; reaction $\Sigma^- \to N\pi^-$ can be considered a transition of the system $\Sigma^- \to N$, and so on. Of course, such formal description does not provide conservation of the energy, unlike, for example, the transition of an electron with spin projection $s_3 = -\frac{1}{2}$ into the state with spin projection $s_3 = +\frac{1}{2}$. From the viewpoint discussed in Chapter 4, transitions $N \to P$, $\Sigma^- \to N$, and so on, can be

considered as quantum transitions of the "octet" whose symmetry is broken by some "internal interaction." The kinematics of the octet, that is, the description of its possible states and transitions, does not change due to this interaction, which is typical for a quantum-mechanical description of interactions.

Let S be the quantum system, that is, its states are represented by vectors of some *linear* space R (in contrast to classical systems whose states are usually described by points of nonlinear phase spaces). Further, space R is *complex*, that is, vectors R can be multiplied by complex numbers. To describe quantitatively the transitions in space R, a positive definite scalar product $\langle\psi|\varphi\rangle$ is introduced to transform R into a *Hilbert space*. Each nonzero vector ψ of R images some state of the system S, the same state is imaged by vectors ψ, $\lambda\psi$ ($\lambda \neq 0$), different states are imaged by noncollinear vectors. Zero-vector images no state of the system and is introduced only for the completeness of mathematical description (so that sums $\psi + \varphi$ and multiples $\lambda\psi$ *always* are possible). If the states ψ, φ are imaged by normalized vectors, that is, $\|\psi\| = 1$, $\|\varphi\| = 1$, the transition probability $\psi \to \varphi$ is $|\langle\psi|\varphi\rangle|^2$.

The kinematics of the system should describe its possible *states* and *transitions*. The set of states is defined by vectors of a Hilbert space R; the transitions are defined by some group of operators which acts in R and is called the *symmetry group* of the system. Thus, a representation of some group G is defined in space R; denote this representation $\{T_g\}$. In our cases, G can be considered a Lie group. The operators of the complex envelope of the Lie algebra $T_A + iT_B$ are assumed to image all possible quantum transitions of the system. If, for example, G contains a subgroup of rotations SO(3), the operators $A_\pm = A_1 \pm iA_2$ translate the vector of the system with quantum number m into the vector with quantum number $m + 1$ or $m - 1$; if G = SU(3), the Okubo operators A_τ^σ translate the octet states into each other (see eq. (4.35) or Appendix B for a more detailed discussion).

If representation $\{T_g\}$ is reducible and R′ is an invariant subspace of R, then the operators of the Lie algebra act within R′ and therefore all possible quantum states of R′ are translated into the states of R′. But then the states of R which do not belong to R′ are unreachable from R′ and there are no reasons to assume that all states of R refer to the *same* quantum system. Therefore, it is natural to assume that representation $\{T_g\}$ is *irreducible*. Thus, the space of state vectors R is the space of the irreducible representation of the symmetry group G. This defines the kinematics of the quantum system.

In the simplest case of complete symmetry, the *dynamics* of the system is also defined by group G. *Observables* of the system are defined by operators T_A to represent Lie algebra of group G. If the observables are to have real eigenvalues, T_A should be Hermitian and, consequently, operators T_g should be *unitary*. So, $\{T_g\}$ is assumed a *unitary representation*. In the case of complete symmetry, the Hamiltonian of the system should commute with all operators T_g, that is, it should be a Casimir operator of group G.

If group G has more than one Casimir operators, additional physical considerations are needed to choose the Hamiltonian.

Of course, the choice of the symmetry group depends on our knowledge. For example, if the electron is not supposed to leave the atom, all electronic states and transitions would be covered by the space of bound electron states (see Chapter 1) with irreducible representation of symmetry group SO(4,2). Or, before SU(3)-symmetry was discovered, isotopic multiplets were considered individual quantum systems, but later they turned out to be part of a wider system with a larger symmetry group.

In the previous discussion, the symmetry group G was interpreted as a group of operators to change the state of the system. But in some cases, the same group describes a variety of systems; for example, the Galilean group (in the nonrelativistic theory) or the Poincare group (in the relativistic theory) describes any free particle; similarly, SU(3) group describes a number of octets and decuplets, baryons and mesons, and so on. In this regard, it is often useful to define group G as a mathematical object (such as a matrix group) independently on the state space of the system; and then, if the group describes transformations of the states, the operators are built to represent the elements of G in the state space of the system. This way the role of *group representations* in quantum mechanics is clarified.

It may happen that a totally symmetric Hamiltonian, that is, a Casimir operator of some group, correctly describes the kinematics but not the dynamics of the system. For the electron in the Coulomb field, it is the Casimir operator of SO(4,2) group (see Section 1.3). Since the whole space of electron states R is irreducible for this group, this Hamiltonian gives the same energy for all electron states, that is, it has a single infinitely degenerate eigenvalue. The electron of the hydrogen atom is never observed in such state of "complete symmetry" which is purely theoretical. In the same way, the "completely symmetric" mass operator of the octet is a Casimir operator of SU(3) group and it has the same value M_0 for all vectors of the eight-dimensional state space; the value M_0 is eightfold degenerate and is never observed experimentally, therefore, the "completely symmetrical" state of the octet is a theoretical construction.

Symmetry breaking can be interpreted as an "activation" of some additional interaction which is assumed much weaker than the one described above and, accordingly, it can cause smaller number of transitions.[42] The transitions possible due to weak interactions are assumed even more possible due to stronger interactions, so some of the previous transitions remain but no new transitions appear. It means that the new interaction is described by a subgroup of G which we denote G_1. The assumption of a weaker nature of this new interaction is mathematically expressed by the fact that besides the "completely symmetrical" Hamiltonian (which commutes with all operators of group G), a much smaller "perturbing" term is also considered to commute

42 This formal interpretation of interactions considers only their relative values rather than their physical nature. The terms "strong interaction" and "weak interaction" are not used and even supposed to be known.

only with subgroup G_1, so the perturbed Hamiltonian of the system also commutes only with G_1. In the case of the electron, perturbation leads to the usual Coulomb Hamiltonian which commutes with subgroup SO(4) but not with SO(4,2). Energy eigenvalues now have finite multiplicities and are observed experimentally. For the octet, the perturbed mass operator no longer commutes with the whole group SU(3) but commutes with the isospin subgroup SU(2). The eigenvalues of the perturbed mass operator (see Section 4.5) have multiplicities 2, 3, 1, 2, but the corresponding states ("isotopic multiplets") are theoretical constructions which are not observed as degenerate states. When a still weaker interaction is turned on, degenerate energy levels of the electron split. In this specific case, the new interaction can actually be added (as a magnetic field). In the case of the octet, the "activation" remains purely theoretical, but the values of the resulting mass operator (without the symmetry) are observed as masses of eight individual particles.

It is natural to assume that operators of the symmetry group or of its subgroup connect similar particle states; if it is a complete symmetry group, the similarity can be manifested in the very possibility of such transition between the states; if it is a subgroup, the possibility of a transition due to *weaker* interaction can be interpreted as a *closer* similarity, so that irreducible representations of a subgroup comprise more similar states or particles. A chain of subgroups leads to a hierarchical classification of states or particles according to the degree of their similarity. Of course, this classification depends on the chosen chain to define the symmetry. If the symmetry is found properly, the above similarity is revealed in physical properties of the particles or the states such as the proximity of energy levels, masses, common values of the observables, regular change of properties within the family of similar states or particles. Such is the case of the hydrogen energy levels split by external magnetic field or of the isotopic mass splitting.

Now we can describe a general scheme to classify the states of a quantum system. To be specific, we will talk about the classification of particles and refer to the mass rather than to the energy.

The *symmetry* is defined by a chain of embedded Lie groups:

$$G = G_0 \supset G_1 \supset G_2 \supset \ldots \supset G_k \tag{4.50}$$

A *system* with this symmetry is defined by an irreducible unitary representation of group G in some Hilbert space R. *Main observables* of the system are obtained as operators of the Lie algebra of group G. Other *observables* of the system are operators to represent the elements of the universal enveloping algebra of group G. The reduction of the representations of group G to subgroup G_1 decomposes R into orthogonal sum of irreducible subspaces of this subgroup $\mathsf{R}_i^{(1)}$:

$$\mathsf{R} = \mathsf{R}_1^{(1)} \oplus \mathsf{R}_2^{(1)} \oplus \cdots \oplus \mathsf{R}_i^{(1)} \oplus \cdots \tag{4.51}$$

The reduction of representation G_1 to subgroup G_2 decomposes subspaces $\mathsf{R}_i^{(1)}$ into irreducible subspaces $\mathsf{R}_{ij}^{(2)}$ of group G_2:

$$\mathsf{R}_i^{(1)} = \mathsf{R}_{i1}^{(2)} \oplus \mathsf{R}_{i2}^{(2)} \oplus \cdots \oplus \mathsf{R}_{ij}^{(2)} \oplus \cdots \tag{4.52}$$

and so on.

Then a maximum system of commuting observables of group G is chosen. Their eigenvalues are called *quantum numbers* of the system. Let quantum numbers be numbered in some order $\lambda_1, \lambda_2, ..., \lambda_l$, so that the set completely defines (up to a factor) the *state vector* of the system $|\lambda_1, \lambda_2, ..., \lambda_l\rangle$ which is an eigenvector for all chosen observables with specified eigenvalues, and such vectors for all possible sets $(\lambda_1, ..., \lambda_l)$ constitute a basis of space R. We call this basis a *distinguished basis*. Assume further that (1) several first quantum numbers $\lambda_1, ..., \lambda_{r_1}$ are the values of the Casimir operators of subgroup G_1, so that all selected basis vectors with these quantum numbers belong to one of the spaces $\mathsf{R}_i^{(1)}$; (2) the following quantum numbers $\lambda_{r_1+1}, ..., \lambda_{r_2}$ are the values of the Casimir operators of subgroup G_2, so that vectors with values $\lambda_1, ..., \lambda_{r_2}$ belong to one of spaces $\mathsf{R}_{ij}^{(2)}$, and so on; and, finally, (3) the last part of quantum numbers in the above sequence defines the position of the vectors of the distinguished basis subgroups in the irreducible subspace of subgroup G_k.

Mass operator is constructed as

$$M = M_0 + M_1 + M_2 + \cdots + M_k + M_{k+1} \tag{4.53}$$

where M_j is a Casimir operator of group G_j ($j = 0,1,\ldots,k$) expressed in terms of the main observables of this group, and M_{k+1} is expressed as a polynomial of the main observables of group G. Operators M_{j+1} are assumed small compared with M_j ($j = 0,1,\ldots,k$), that is, matrix elements M_{j+1} are small compared with matrix elements M_j.

Elementary particles are states with definite masses, that is, their vectors are eigenvectors of the mass operator. The corresponding eigenvalues are assumed nondegenerate (i.e. there is a single particle of the given mass).[43]

The distinguished basis can usually be chosen to make mass eigenvectors close to the vectors of the distinguished basis. Suppose (in some approximation) that states with a definite mass value are *defined* by the vectors of the distinguished basis. Then, replacing the main observables in the expression of operator M by corresponding eigenvalues of these observables, particle masses are expressed as polynomials of quantum numbers λ_j; this expression is called the *mass formula* and is usually used instead of eq. (4.53) to express the mass operator in terms of the operators of observables. *Thus, masses of particles depend on their quantum numbers*. If the symmetry of system (eq. (4.50)) is found properly, any other measurable property of particles P can also be assumed to depend on quantum numbers, that is, there is a quite regular relationship

43 This assumption is sufficient for our further purposes but unnecessary in the general case. We will discuss this point below.

$$P = P(\lambda_1, \dots, \lambda_l) \tag{4.54}$$

All particles of the system constitute a *multiplet* of group G. Particles with state vectors belonging to the irreducible subspace $\mathsf{R}_j^{(1)}$ of subgroup G_1 constitute a multiplet of this subgroup, and so on. The correctness of this "hierarchical" classification is confirmed by similar particle properties within "small" multiplets in contrast to "big" multiplets; the similarity is not necessarily to be *quantitative*, rather, it is a *regularity in the change of their properties* within the multiplet and its lack beyond the multiplet. So, the proximity of masses and regular charge changes are observed within isotopic multiplets. Below a number of examples will be discussed to illustrate the classification of chemical elements.

If the mass operator has degenerate eigenvalues, then state vectors of individual particles are characterized by a set of quantum numbers λ_j. This is the case of the hydrogen atom where the degeneracy of energy eigenvalues makes it necessary to use orbital angular momentum L^2 and its projection L_z to characterize the states. Of course, such description of states implies some arbitrariness (for example, the choice of L_z instead of L_x or L_y).

Some particles of the system may happen to have very similar properties even though they belong, according to the group classification, to different multiplets of the chain of subgroups (4.50). Such particles whose "similarity" is not associated with the "easiness of transitions" within small multiplets are called the *homologs* of the system. For SU(6) symmetry, the states of the 56-plet or the 35-plet which differ only by the projection of the (usual) spin (see Section 3.6), are homologs. A simple principle to distinguish homologous series is as follows (see Fet, 1975, p. 326). Suppose homologous particles in the multiplets of subgroup G_i are to be found. Assume that the Lie algebra of group G contains operator Γ which translates homologous state vectors into each other, for example, $v_2 = \Gamma v_1$, where v_j belongs to the j-th multiplet ($j = 1,2$). If A is an operator of the Lie algebra of subgroup G_i, the vectors $v_i' = Av_1$ and $v_2' = Av_2$ can be assumed, due to their similar algebraic connection with v_1, v_2 in the corresponding multiplets, to be also homologous relative to each other. But then $v_2' = \Gamma v_1'$, that is, $A\Gamma v_1 = \Gamma A v_1$. If each particle belongs to some homologous series, then for v_1, any basis vector can be chosen; therefore, $A\Gamma = \Gamma A$, that is, *operator* Γ *commutes with all operators of subgroup* G_j. Such operators are called *affinity operators*.

"Superposition principle" for our systems is understood only in the sense that the spaces of state vectors are linear but not in the usual sense that superposition of physically possible states is a physically possible state. For example, a linear combination of the proton state of the neutron state does not correspond to any physical state of the octet. Only individual states corresponding to individual values of masses are real; in this sense, the systems considered in the particle classification are the extreme case of Wigner's "superselection principle."

5 The symmetry group of chemical elements

5.1 Description of the system of elements

Dmitri Mendeleev was the first to suggest that properties of the atoms depend on their positions in the whole integral system they form. If atoms are arranged in the order of increasing atomic weights, their chemical properties change periodically and homologous series of elements with similar properties can be identified. Thus, the first classification of particles originated long before the beginning of atomic physics when the very concepts of the atom and the molecule were challenged say nothing of any physical explanation of these regularities.

Such explanation was suggested in 1921 by Bohr who based it on his theory of atom suggested in 1911 and later developed by other authors, especially by Sommerfeld. At present, this theory is known as the "old quantum mechanics." After the creation of modern quantum mechanics (1925–1926), the arrangement of elements proposed by Bohr was interpreted in terms of many-electron Schrödinger equation and lead to the so-called "model of electron shells." That is how *Bohr's model* was born which is now a conventional tool to describe the atoms.

To understand the following ideas, the relation between the group description of elements and the Bohr's model is to be clarified and its place in quantum mechanics is to be discussed.

As is known, multielectron Schrodinger equation allows no exact solution, and all its consequences are obtained approximately based on simplifications. Bohr's model assumes each electron is in a central field made up of the Coulomb field of the nucleus and the fictitious field of a spherically symmetric charged shell used to describe the total charge of all other electrons. Such replacement is intuitively justified by the idea that electrons move within the atom sufficiently fast and quite independently of each other and form a continuous charge distribution to "shield" the nucleus while the "isolated" electron moves in this field. Since the positions of individual electrons are believed to be almost independent, the distribution of such fictitious charge should not have privileged directions, so its density can be assumed spherically symmetric. Of course, distinguishing between the "isolated" and "the other" electrons is a purely theoretical construction which contradicts the principle of electrons undistinguishability, and therefore it is to be corrected, which will be done later when discussing the Pauli exclusion principle. This assumption allows describing the electron in a multielectron atom like that in a hydrogen atom and the exact solution of the Schrödinger equation can be obtained. Stationary states of this "hydrogen" electron are described by quantum numbers n, l, m and the "spin projection" $s = \pm\frac{1}{2}$ suggested in 1925 by Pauli.

Then Pauli principle is applied to this to prohibit two different electrons occupy the same state. The Pauli principle is considered a general law of nature, but its

application in each case requires a correct description of possible states, that is, kinematics of the quantum system. It is assumed that, though the systems are different, the electron states in both multielectron atom and in one-electron atom are correctly described by the same set of quantum numbers n, l, m, and s. This way Pauli principle makes it possible a step-by-step procedure to fill electron shells.

A classical description of this procedure can be found in Sommerfeld's treatise (Sommerfeld, 1923, vol. 1, ch. 3), where the procedure was shown to describe successfully spectra and chemical properties of elements in accordance with the Bohr's model. However, this model is not a logical consequence of general principles of quantum mechanics and the idea that atom consists of nuclei and electrons. It was evident for the founders of quantum mechanics; in particular, Sommerfeld emphasizes twice a "somewhat cabalistic" nature of the above procedure (Sommerfeld, 1923, vol. 1, ch. 3, paragraphs 3–4). From the viewpoint of modern quantum mechanics, Bohr's model should be regarded as an *approximate method* to solve the multielectron Schrödinger equation. These remarks, of course, in no way diminish the significance of Bohr's model and have the only goal to remind that it is not a single logically possible description of the elements consistent with the principles of quantum mechanics.

Evidently, Bohr's model does not describe the atoms of different elements as a single quantum system. In fact, the concept of a quantum system assumes a Hilbert space whose vectors represent all possible states of the system, and a Hamiltonian defined on this space whose eigenvectors represent stationary states of the system; in this case, these states should represent the atoms of all elements. Bohr's model lacks such description (which was not possible before the ideas of isospin and unitary symmetry were suggested); moreover, Bohr's model has no symmetry group operators to carry into each other state vectors corresponding to different elements. Quantum system considered in the Bohr's model is an atom of a *single* fixed element with a given atomic number Z; stationary states of the system are different energy states of *the same* atom. The atomic number Z is not a quantum number of the theory, but a *parameter* in the multielectron Schrödinger equation, and the task of the Bohr's model is to find the approximate solution of this equation. A stable state of the atom is described as a state with the lowest energy, and then such states of *different* quantum systems with different Z values are arranged into ascending order of energy.

Numbers n, l, m, and s are not quantum numbers in Bohr's model in the sense defined in Chapter 2; these numbers define the states of a single atomic electron, whereas numbers n, and l may serve to label electron shells. Since Bohr's model does not comprise any integral quantum-mechanical description of elements, it numerates the elements by means of the atomic number Z to separate atoms as individual quantum systems rather than to unify them. As to numbers n, l, m, and s, they cannot serve in Bohr's model to numerate elements and are not used as such (Sommerfeld, 1923).

The first attempt to apply the "hydrogen" quantum numbers n, l, m, and s to number the elements was made by Madelung who noticed in the 1920s that these numbers are convenient classification of elements according to their properties. Since this numbering had no theoretical justification, Madelung called it "empirical"; in particular, he could not relate it to Bohr's model. Perhaps for this reason, he published it in an unusual way, in his Reference Book on mathematical methods of physics which run into several editions (Madelung, 1964).[44] However, the table in Madelung (1964) says nothing about the nature of the Madelung numbers.

Compare Madelung numeration with Table 5.1 cited from the paper written by Rumer and Fet in (1971). Columns of the table define value n, rows define values l and m. For example, M_n corresponds to $n = 3$, $l = 2$, $m = 0$. Each triplet n, l, m corresponds to a pair of elements designated by the number $s = \pm 1/2$; so, M_n is numbered by values $(3,2,0,-1/2)$, Fe by $(3,2,0,1/2)$. Numbers n, l, m, s in Table 5.1 do not coincide with those of Madelung but are related to them by a simple change of variables. The ranges for the numbers are as follows:

$$\begin{aligned} & n = 1, 2, \dots ; \\ \text{for given } n: \quad & l = 0, 1, \dots, n-1; \\ \text{for given } n, l: \quad & m = -l, -l+1, \dots, l-1, l; \\ \text{for given } n, \ l, \ m: \quad & s = -1/2, 1/2. \end{aligned} \tag{5.1}$$

Now compare Table 5.1 with Table 1.1 to represent the basis of some irreducible representation of the conformal group SO(4,2). As is easily seen, numbers n, l, m vary within the same limits in both tables. This suggests the idea that the system of elements is related to this special representation of the conformal group which was used in Chapter 1 to describe energy spectrum of the hydrogen atom. Mendeleevian homologous series make rows in Table 5.1, that is, they are obtained for fixed l, m, s, and varied n. This indicates that Madelung numbers and, therefore, the conformal group are closely related to chemical properties of the elements.

However, the realization of the plan meets two obstacles. First, the Madelung number s is in no way related to the conformal group and needs to be explained. Each basis vector of the representation in Table 5.1 (identical to the initial table proposed by Rumer in 1970) is associated with *two* elements rather than with one element. Further, as we will see, the properties of the elements depend on $n + l$ rather than on Madelung numbers n, l as such. But before we proceed to construct the symmetry group and the representation, explain the fundamental meaning of this theory.

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44 The author learned about Madelung's numeration only at a late stage of the work, after Fet (1975) had been published. The numeration in Fet (1975), essentially identical to that of Madelung, was suggested by Yuriy Kulakov (Byakov et al., 1976). In this book, we do not follow our original line of thought; rather, we start with the Madelung numbers to facilitate understanding of the method to be described below.

Table 5.1: Periodic table from the paper by Rumer and Fet (1971).

	$n=1$	$n=2$	$n=3$	$n=4$	$n=5$	$n=6$	$n=7$	
$l=0$	H He	Li He	Na Mg	K Ca	Rb Sr	Cs Ba	Fr Ra	$m=0$
		B C	Al Si	Ga Ge	In Sn	Ti Pb		$m=-1$
$l=1$		N O	P S	As Se	Sb Te	Bi Po		$m=0$
		F Ne	Cl Ar	Br Kr	J Xe	At Rn		$m=1$
		$g=-½$ $k=½$	Sc Ti	Y Zr	Lu Hf	Lr Ku		$m=-2$
			V Cr	Nb Mo	Ta W			$m=-1$
$l=2$			Mn Fe	Tc Ru	Re Os			$m=0$
			Co Ni	Rb Pd	Ir Pt			$m=1$
			Cu Zn	Ag Cd	Au Hg			$m=2$
				La Ce	Ac Th			$m=-3$
				Pr Nd	Pa U			$m=-2$
				Pm Sm	Np Pu			$m=-1$
$l=3$				Eu Gd	Am Cm			$m=0$
				Tb Dy	Bk Cf			$m=1$
				Ho Er	Es Fm			$m=2$
				Tm Yb	Md No			$m=3$

The atoms of all possible elements are assumed to form a multiplet of a certain symmetry group G in the sense discussed in Section 4.7, that is, they correspond to the eigenvectors of some mass operator defined in the space of an irreducible representation of group G. Then a chain of imbedded subgroups (eq. (4.50)) is constructed to define the symmetry of the corresponding quantum system. The reduction of the representation of group G upon these subgroups divides the multiplet of all elements into smaller multiplets, which are found to be natural families of elements and thus define a classification of the element. Therefore, atoms of all elements are described

as an *integral quantum system* similar to the multiplets of the unitary symmetry (in contrast to Bohr's model).

This description was first proposed in 1971 by Rumer and Fet, where the representation space corresponding to Table 5.1 was already constructed, but SU(2) × SO(4) group was taken as a group symmetry. Konopelchenko (1972) introduced SO(4,2) as a symmetry group for elements by extending Fock's representation to the representations of the conformal group; this extension was applied previously to the hydrogen atom in Malkin and Manko (1965). The conformal group was independently proposed to describe the elements by Barut (1972) and Novaro and Barrondo (1972); however, the approach of these authors differs from ours: they considered the symmetry as a symmetry of electronic shells without distinguishing it from the Bohr's model. Meanwhile, a different point of view was formulated in Rumer and Fet (1971) where it was clearly stated that the suggested symmetry is the symmetry of the *system of atoms as a whole*. This interpretation, developed by the author in Fet (1974, 1975) and Byakov et al. (1976), is confirmed by mass formula to describe atomic weights (Fet, 1979a,1979b, 1981). Further, the chain of symmetry groups built in these studies has also advantages as far as revealing some previously unseen experimental regularities in chemical properties.

The representation of the symmetry group to describe the elements is of infinite dimension; this means that the number of elements is assumed infinite. It is not a contradiction because elements with high quantum numbers are unstable and are not met in nature. For example, in SU(3) symmetry, only the dimensions 8 and 10 are realized from all theoretical possibilities 8, 10, 27, 35, … Stability of the particles is not the subject to such theories. We note only that our system does not distinguish isotopes of elements and provides no quantum numbers for them.

Note that the proposed model "ignores" the *structure* of atoms which underlies Bohr' model. Evidently, all information depending on the atomic structure is lost, but some new information hidden by the complex picture of the electron shells can be obtained. Moreover, the mass formula and some other results relate to atomic nuclei rather than to Bohr's model. Applying the same group approach to the atoms and to "elementary" particles can hardly draw objections: now hadrons are also known to have a complex structure. As shown in Chapter 4, the very concept of elementary particles depends on the symmetry group underlying the description.

In the conventional language of the structural theory, our symmetry describes both the nuclei and the electron shells; it may seem strange as nuclear and Coulomb forces differ in nature and magnitude. However, the theory describes (in terms of the structural theory) the symmetry of certain *configurations* of nucleons and electrons rather than the symmetry of nuclear or Coulomb fields. Naturally, any symmetry of nuclear configurations should call forth a similar symmetry of electron shells: as Sommerfeld emphasized, "*the structure of atom from its interior to the periphery is uniquely defined by the value of the nuclear charge*" (Sommerfeld, 1923, vol. 1, Ch. 3, Section 13).

Though the same (conformal) group is used to describe the hydrogen atom and the system of elements, it does not mean that the theory is the same. Conformal group is often used in modern physics and seems to be as universal as the Lorentz group;

there is a lot of conformal and relativistic theories. In the conformal group, there are "raising" and "lowering" the operators of Lie algebra, similar to $L_{\pm} = L_1 \pm iL_2$; but in the case of the hydrogen atom, they carry into each other different excited states of the electron, whereas in our case, they work on the *atoms of different elements*.

Hence, the most important difference between the proposed model and Bohr's model is that the latter considers a quantum system as an atom of *a single element* (with atomic number used in the theory as a parameter, so there are as many quantum systems as elements) while in our model atoms of all elements are considered as the states of an integrated quantum system connected by actions of a symmetry group.

5.2 The conformal group

Consider a six-dimensional space R^6 with real coordinates $\xi_1, \dots, \xi_6$. All linear homogeneous transformations

$$\begin{aligned} \xi'_1 &= c_{11}\xi_1 + \cdots + c_{16}\xi_6 \\ &\cdots\cdots\cdots\cdots\cdots\cdots \\ \xi'_6 &= c_{16}\xi_1 + \cdots + c_{66}\xi_6 \end{aligned} \tag{5.2}$$

preserving the quadratic form

$$Q(\xi_1, \dots, \xi_6) = \xi_1^2 + \xi_2^2 + \xi_3^2 + \xi_4^2 - \xi_5^2 - \xi_6^2 \tag{5.3}$$

that is, such that

$$Q(\xi'_1, \dots, \xi'_6) = Q(\xi_1, \dots, \xi_6) \tag{5.4}$$

constitute a group denoted O(4,2). The subgroup of O(4,2) composed of all transformations with determinant 1 is called a *conformal group* and is denoted SO(4,2). Write the form (5.3) as

$$Q(\xi) = \sum_{\alpha,\beta=1}^{6} g_{\alpha\beta}\xi_\alpha\xi_\beta \tag{5.5}$$

where

$$g_{11} = g_{22} = g_{33} = g_{44} = 1, g_{55} = g_{66} = -1 \tag{5.6}$$

Then the condition (5.4) takes the form

$$\sum_{\alpha,\beta=1}^{6} g_{\alpha\beta}\xi'_\alpha\xi'_\beta = \sum_{y,\delta=1}^{6} g_{y\delta}\xi_y\xi_\delta \tag{5.7}$$

or, from eq. (5.2)

$$\sum_{\alpha,\beta,y,\delta=1}^{6} g_{\alpha\beta}c_{\alpha y}c_{\beta\delta}\xi_y\xi_\delta = \sum_{y,\delta=1}^{6} g_{y\delta}\xi_y\xi_\delta \tag{5.8}$$

Since this equation must be identical with respect to ξ_y, it is equivalent to

$$g_{y\delta} = \sum_{\alpha,\beta=1}^{6} g_{\alpha\beta} c_{\alpha y} c_{\beta\delta} \tag{5.9}$$

or, in the matrix form:

$$G = {}^tCGC \tag{5.10}$$

Since the determinant of the product of matrices is the product of their determinants, from $\det|G| = 1$ and $\det|{}^tC| = \det|C|$ obtain that $|\det C|^2 = 1$, that is,

$$\det|C| = \pm 1 \tag{5.11}$$

for all transformations C of the group O(4,2).

Since one-parametric subgroups $O(4,2)$ consist of matrices C_α continuous in α, $\det|C_\alpha| = \det|C_0| = \det|1| = 1$. So all these subgroups belong to SO(4,2), and the Lie algebra of this subgroup coincides with that of the whole group (like in the case of SO(n)). To find this Lie algebra, write these one-parametric subgroups in the form (3.31):

$$C_\alpha = e^{-i\alpha A} \tag{5.12}$$

where A belongs to the Lie algebra. Then from eq. (5.10), it follows

$${}^tC_\alpha^{-1} = e^{i\alpha {}^tA} = Ge^{-i\alpha A}G^{-1} \tag{5.13}$$

or

$$1 + i\alpha {}^tA + \cdots = 1 - i\alpha GAG^{-1} + \cdots \tag{5.14}$$

where the dots denote the higher order terms in α, whence

$${}^tA = -GAG^{-1} \tag{5.15}$$

This condition, similar to the antisymmetric property of the orthogonal group, completely defines the Lie algebra of the conformal group. We write it as

$$a_{\beta\alpha} = -\sum_{y,\delta=1}^{6} g_{\alpha y} a_{y\delta} g^{-1}_{\delta\beta} \tag{5.16}$$

Since $G^{-1} = G$ and $g_{\alpha y} = g_{\alpha\alpha}\delta_{\alpha y}$, this is equivalent to

$$a_{\beta\alpha} = \sum_{y,\delta=1}^{6} g_{\alpha\alpha}\delta_{\alpha y} a_{y\delta}\delta_{\delta\beta} g_{\beta\beta} = -g_{\alpha\alpha} a_{\alpha\beta} g_{\beta\beta} \tag{5.17}$$

So $a_{\alpha\alpha} = 0$, and the matrix A is completely determined by the elements above its main diagonal. Therefore, the dimension of SO(4,2) is 15, which is the number of generators of its Lie algebra.

It is easy to find a simple system of generators corresponding to 15 one-parameter subgroups. The subgroups of rotations in the planes $(\xi_\alpha \xi_\beta)$, $1 \le \alpha < \beta \le 4$ of the form

$$\begin{aligned}\xi'_\alpha &= \xi_\alpha \cos\alpha - \xi_\beta \sin\alpha \\ \xi'_\beta &= \xi_\alpha \sin\alpha + \xi_\beta \cos\alpha \\ \xi'_x &= \xi_x (x \neq \alpha, \beta)\end{aligned} \tag{5.18}$$

correspond, as in the case of orthogonal groups, to the generators $L_{\alpha\beta}$ with two nonzero elements: $(L_{\alpha\beta})_{\alpha\beta} = -i$ and $(L_{\alpha\beta})_{\beta\alpha} = i$; or

$$(L_{\alpha\beta})_{\sigma\tau} = -i(\delta_{\alpha\sigma}\delta_{\beta\tau} - \delta_{\beta\sigma}\delta_{\alpha\tau})(\alpha, \beta = 1, ..., 4, \alpha < \beta) \tag{5.19}$$

The subgroups of transformations in the planes $(\xi_y \xi_\delta)$, $1 \le y \le 4$, $\delta = 5, 6$, preserving $\xi_y^2 - \xi_\delta^2$ and having the form (see eq. (2.26))

$$\begin{aligned}\xi'_y &= \xi_y ch\alpha - \xi_\delta sh\alpha \\ \xi'_\delta &= \xi_y sh\alpha + \xi_\delta ch\alpha \\ \xi'_x &= \xi_x \ (x \neq y, \delta)\end{aligned} \tag{5.20}$$

correspond to the generators $L_{y\delta}$ with nonzero elements $(L_{y\delta})_{y\delta} = i$ and $(L_{y\delta})_{\delta y} = i$; that is,

$$(L_{y\delta})_{\sigma\tau} = i(\delta_{y\sigma}\delta_{\delta\tau} - \delta_{\delta\sigma}\delta_{y\tau})(y = 1, \dots, 4, \delta = 5, 6) \tag{5.21}$$

Finally, the one-parametric subgroup of rotations in the plane $(\xi_5 \xi_6)$, written for simplification as

$$\begin{aligned}\xi'_5 &= \xi_5 \cos\alpha + \xi_6 \sin\alpha \\ \xi'_6 &= -\xi_5 \sin\alpha + \xi_6 \cos\alpha\end{aligned} \tag{5.22}$$

(changing the sign of α as compared to eq. (5.18)), corresponds to the generator L_{56} with nonzero elements $(L_{56})_{56} = i$, $(L_{56})_{65} = -i$; that is,

$$(L_{56})_{\sigma\tau} = i(\delta_{5\sigma}\delta_{6\tau} - \delta_{6\sigma}\delta_{5\tau}) \tag{5.23}$$

The number of operators (5.19), (5.21), and (5.23) is 6, 8, and 1, respectively, so that their total is 15; it readily verified that they are linearly independent. Since the dimension of the group and, therefore, of the Lie algebra, is 15, we have a complete system of generators of SO(4,2).

Now, define matrices $L_{\alpha\beta}$ with $\alpha > \beta$ by

$$L_{\alpha\beta} = -L_{\beta\alpha} 1 \le \beta < \alpha \le 6 \tag{5.24}$$

and note that eqs. (5.19) and (5.23) are true for these matrices, and eq. (5.21) is true if the sign is changed. Then the following commutation relations are evidently true:

$$\begin{aligned}&[L_{\alpha\beta}, L_{y\delta}] = i(g_{\alpha y}L_{\beta\delta} + g_{\beta\delta}L_{\alpha y} - g_{\alpha\delta}L_{\beta y} - g_{\beta y}L_{\alpha\delta}) \\ &(\alpha, \beta, y, \delta = 1, \dots, 6, \alpha \neq \beta, y \neq \delta)\end{aligned} \tag{5.25}$$

We perform the calculations for $1 \le \alpha, \beta, y, \delta \le 4$ and leave the remaining cases to the reader. It is sufficient to assume $\alpha < \beta, y < \delta$, since other possibilities are reduced to this one using eq. (5.24). From eq. (5.19), we have

$$(L_{\alpha\beta}L_{y\delta})_{\sigma\tau} = \sum_{\rho=1}^{6}(L_{\alpha\beta})_{\sigma\rho}(L_{y\delta})_{\rho\tau} = -\sum_{\rho=1}^{6}(\delta_{\alpha\sigma}\delta_{\beta\rho} - \delta_{\beta\sigma}\delta_{\alpha\rho})(\delta_{y\rho}\delta_{\delta\tau} - \delta_{\delta\rho}\delta_{y\tau}) \tag{5.26}$$

Removing the brackets and using identities like $\sum_{\rho=1}^{6}\delta_{\alpha\rho}\delta_{y\rho} = \delta_{\alpha y}$, we get

$$-\delta_{\alpha\sigma}\delta_{\beta y}\delta_{\delta\tau} + \delta_{\alpha\sigma}\delta_{\beta\delta}\delta_{y\tau} + \delta_{\beta\sigma}\delta_{\alpha y}\delta_{\delta\tau} - \delta_{\beta\sigma}\delta_{\alpha\delta}\delta_{y\tau} \tag{5.27}$$

The elements of the matrix $L_{y\delta}L_{\alpha\beta}$ are obtained by substituting y, δ instead of α, β, and vice versa. Subtracting these elements from eq. (5.27) and using eq. (5.19), we find

$$[L_{\alpha\beta}, L_{y\delta}] = i(-\delta_{\beta y}L_{\alpha\delta} - \delta_{\alpha\delta}L_{\beta y} + \delta_{\beta\delta}L_{\alpha y} + \delta_{\alpha y}L_{\beta\delta}) \tag{5.28}$$

which coincides with eq. (5.25), as $g_{\alpha\beta} = \delta_{\alpha\beta}$ *for* $1 \le \alpha, \beta \le 4$.

Further generators $L_{\alpha\beta}$ and their commutation relations will be used to construct representations of the group SO(4,2) as described in Section 3.3. It will be more convenient to use the system of generators suggested by Yao (1967) instead of the "simplest" generators. Take the 18 matrices

$$\begin{aligned}
&J_1 = \frac{1}{2}(L_{23} - L_{14}), \quad J_2 = \frac{1}{2}(L_{31} - L_{24}), \quad J_3 = \frac{1}{2}(L_{12} - L_{34})\\
&K_1 = \frac{1}{2}(L_{23} + L_{14}), \quad K_2 = \frac{1}{2}(L_{31} + L_{24}), \quad K_3 = \frac{1}{2}(L_{12} + L_{34})\\
&P_1 = \frac{1}{2}(-L_{35} - L_{46}), \quad P_2 = \frac{1}{2}(L_{45} - L_{36}), \quad P_0 = \frac{1}{2}(-L_{34} - L_{56})\\
&Q_1 = \frac{1}{2}(L_{35} - L_{46}), \quad Q_2 = \frac{1}{2}(L_{45} + L_{36}), \quad Q_0 = \frac{1}{2}(L_{34} - L_{56})\\
&S_1 = \frac{1}{2}(-L_{15} + L_{26}), \quad S_2 = \frac{1}{2}(-L_{25} - L_{16}), \quad S_0 = \frac{1}{2}(L_{12} - L_{56})\\
&T_1 = \frac{1}{2}(-L_{15} - L_{26}), \quad T_2 = \frac{1}{2}(L_{25} - L_{16}), \quad T_0 = \frac{1}{2}(-L_{12} - L_{56})
\end{aligned} \tag{5.29}$$

connected by three relations

$$J_3 - K_3 = P_0 - Q_0, \quad J_3 + K_3 = S_0 - T_0, \quad P_0 + Q_0 = S_0 + T_0. \tag{5.30}$$

Since generators $L_{\alpha\beta}(\alpha < \beta)$ are independent, matrices (5.29) form a "redundant" system of generators of group SO(4,2) from which a basis of the Lie algebra is obtained by eliminating three generators using eq. (5.30). The commutation relations for the generators (eq. (5.29)) are obtained from eq. (5.25) by apparent though somewhat tiresome calculations. They are more convenient written for the operators of the complex envelope of the Lie algebra. If we define

$$
\begin{aligned}
J_\pm &= J_1 \pm iJ_2 \qquad P_\pm = P_1 \pm iP_2 \qquad S_\pm = S_1 \pm iS_2 \\
K_\pm &= K_1 \pm iK_2 \quad Q_\pm = Q_1 \pm iQ_2 \quad T_\pm = T_1 \pm iT_2
\end{aligned}
\tag{5.31}
$$

then

$$
\begin{aligned}
&[J_3, J_+] = J_+ \qquad [J_3, J_-] = -J_- \qquad [J_+, J_-] = 2J_3 \\
&[K_3, K_+] = K_+ \qquad [K_3, K_-] = -K_- \qquad [K_+, K_-] = 2K_3 \\
&[P_0, P_+] = P_+ \qquad [P_0, P_-] = -P_- \qquad [P_+, P_-] = -2P_0 \\
&[Q_0, Q_+] = Q_+ \qquad [Q_0, Q_-] = -Q_- \qquad [Q_+, Q_-] = -2Q_0 \\
&[S_0, S_+] = S_+ \qquad [S_0, S_-] = -S_- \qquad [S_+, S_-] = -2S_0 \\
&[T_0, T_+] = T_+ \qquad [T_0, T_-] = -T_- \qquad [T_+, T_-] = -2T_0 \\
&[J_i, K_j] = 0 (i, j = +, -, 3)
\end{aligned}
$$

$$
\begin{aligned}
&[J_+, P_+] = 0 \qquad [J_+, P_-] = -T_- \qquad [J_+, P_0] = -\frac{1}{2}J_+ \\
&[J_-, P_+] = T_+ \qquad [J_-, P_-] = 0 \qquad [J_-, P_0] = \frac{1}{2}J_- \\
&[J_3, P_+] = \frac{1}{2}P_+ \qquad [J_3, P_-] = -\frac{1}{2}P_- \qquad [J_3, P_0] = 0 \\
&[J_+, Q_+] = S_+ \qquad [J_+, Q_-] = 0 \qquad [J_+, Q_0] = \frac{1}{2}J_+ \\
&[J_-, Q_+] = 0 \qquad [J_-, Q_-] = -S_- \qquad [J_-, Q_0] = -\frac{1}{2}J_- \\
&[J_3, Q_+] = -\frac{1}{2}Q_+ \qquad [J_3, Q_-] = \frac{1}{2}Q_- \qquad [J_3, Q_0] = 0 \\
&[J_+, S_+] = 0 \qquad [J_+, S_-] = -Q_- \qquad [J_+, S_0] = -\frac{1}{2}J_+ \\
&[J_-, S_+] = Q_+ \qquad [J_-, S_-] = 0 \qquad [J_-, S_0] = \frac{1}{2}J_- \\
&[J_3, S_+] = \frac{1}{2}S_+ \qquad [J_3, S_-] = -\frac{1}{2}S_- \qquad [J_3, S_0] = 0 \\
&[J_+, T_+] = P_+ \qquad [J_+, T_-] = 0 \qquad [J_+, T_0] = \frac{1}{2}J_+ \\
&[J_-, T_+] = 0 \qquad [J_-, T_-] = -P_- \qquad [J_-, T_0] = -\frac{1}{2}J_- \\
&[J_3, T_+] = -\frac{1}{2}T_+ \qquad [J_3, T_-] = \frac{1}{2}T_- \qquad [J_3, T_0] = 0 \\
&[K_+, P_+] = -S_+ \qquad [K_+, P_-] = 0 \qquad [K_+, P_0] = \frac{1}{2}K_+ \\
&[K_-, P_+] = 0 \qquad [K_-, P_-] = S_- \qquad [K_-, P_0] = -\frac{1}{2}K_- \\
&[K_3, P_+] = -\frac{1}{2}P_+ \qquad [K_3, P_-] = \frac{1}{2}P_- \qquad [K_3, P_0] = 0
\end{aligned}
\tag{5.32}
$$

$$[K_+, Q_+] = 0 \qquad [K_+, Q_-] = T_- \qquad [K_+, Q_0] = -\frac{1}{2}K_+$$

$$[K_-, Q_+] = -T_+ \qquad [K_-, Q_-] = 0 \qquad [K_-, Q_0] = \frac{1}{2}K_-$$

$$[K_3, Q_+] = \frac{1}{2}Q_+ \qquad [K_3, Q_-] = -\frac{1}{2}Q_- \qquad [K_3, Q_0] = 0$$

$$[K_+, S_+] = 0 \qquad [K_+, S_-] = P_- \qquad [K_+, S_0] = -\frac{1}{2}K_+$$

$$[K_-, S_+] = -P_+ \qquad [K_-, S_-] = 0 \qquad [K_-, S_0] = \frac{1}{2}K_-$$

$$[K_3, S_+] = \frac{1}{2}S_+ \qquad [K_3, S_-] = -\frac{1}{2}S_- \qquad [K_3, S_0] = 0$$

$$[K_+, T_+] = -Q_+ \qquad [K_+, T_-] = 0 \qquad [K_+, T_0] = \frac{1}{2}K_+$$

$$[K_-, T_+] = 0 \qquad [K_-, T_-] = Q_- \qquad [K_-, T_0] = -\frac{1}{2}K_-$$

$$[K_3, T_+] = -\frac{1}{2}T_+ \qquad [K_3, T_-] = \frac{1}{2}T_- \qquad [K_3, T_0] = 0$$

$$[P_i, Q_j] = 0 (i, j = +, -, 0)$$

$$[P_+, S_+] = 0 \qquad [P_+, S_-] = K_- \qquad [P_+, S_0] = -\tfrac{1}{2}P_+$$

$$[P_-, S_+] = -K_+ \qquad [P_-, S_-] = 0 \qquad [P_-, S_0] = \tfrac{1}{2}P_-$$

$$[P_0, S_+] = \tfrac{1}{2}S_+ \qquad [P_0, S_-] = -\tfrac{1}{2}S_- \qquad [P_0, S_0] = 0$$

$$[P_+, T_+] = 0 \qquad [P_+, T_-] = -J_+ \qquad [P_+, T_0] = -\tfrac{1}{2}P_+$$

$$[P_-, T_+] = J_- \qquad [P_-, T_-] = 0 \qquad [P_-, T_0] = \tfrac{1}{2}P_-$$

$$[P_0, T_+] = \tfrac{1}{2}T_+ \qquad [P_0, T_-] = -\tfrac{1}{2}T_- \qquad [P_0, T_0] = 0$$

$$[Q_+, S_+] = 0 \qquad [Q_+, S_-] = -J_- \qquad [Q_+, S_0] = -\tfrac{1}{2}Q_+$$

$$[Q_-, S_+] = J_+ \qquad [Q_-, S_-] = 0 \qquad [Q_-, S_0] = \tfrac{1}{2}Q_-$$

$$[Q_0, S_+] = \tfrac{1}{2}S_+ \qquad [Q_0, S_-] = -\tfrac{1}{2}S_- \qquad [Q_0, S_0] = 0$$

$$[Q_+, T_+] = 0 \qquad [Q_+, T_-] = K_+ \qquad [Q_+, T_0] = -\tfrac{1}{2}Q_+$$

$$[Q_-, T_+] = -K_- \qquad [Q_-, T_-] = 0 \qquad [Q_-, T_0] = \tfrac{1}{2}Q_-$$

$$[Q_0, T_+] = \tfrac{1}{2}T_+ \qquad [Q_0, T_-] = -\tfrac{1}{2}T_- \qquad [Q_0, T_0] = 0$$

$$[S_i, T_j] = 0 (i, j = +, -, 0)$$

Transformations (5.2) preserving ξ_5, ξ_6, that is, such that $\xi'_5 = \xi_5, \xi'_6 = \xi_6$, have matrices C with elements $c_{56} = c_{65} = 0$, $c_{55} = c_{66} = 1$, $c_{5\beta} = c_{6\beta} = 0 (1 \le \beta \le 4)$. From eqs. (5.9) and (5.6), it follows that

$$\sum_{\alpha=1}^{4} c_{\alpha y}^2 - 1 = -1 \quad \text{for } y = 5, 6, \tag{5.33}$$

So that $c_{\alpha\gamma} = 0 (1 \le \alpha \le 4, \gamma = 5, 6)$. Thus, the matrix C has the form

$$C = \left[\begin{array}{c|cc} c_{\alpha\beta} & \multicolumn{2}{c}{0} \\ \hline 0 & 1 & 0 \\ & 0 & 1 \end{array}\right] \tag{5.34}$$

and from eq. (5.3) follows that matrix $(c_{\alpha\beta})(1 \le \alpha, \beta \le 4)$ preserves the form $\xi_1^2 + \xi_2^2 + \xi_3^2 + \xi_4^2$. Therefore, the subgroup of transformations to preserve ξ_5, ξ_6 is found to be in a one to one correspondence with the group matrices of fourth order SO(4), so that multiplication of matrices (5.34) corresponds to multiplication in SO(4). This means that the above subgroup is isomorphic to SO(4), and we denote it simply SO(4). Its Lie algebra is generated by one-parametric subgroups of rotations in the planes $(\xi_\alpha \xi_\beta)(1 \le \alpha, \beta \le 4)$; that is, it has generators $L_{\alpha\beta}$ with the same indices. Instead of these, we can take linear combinations $J_k, K_k (k = 1, 2, 3)$ defined in eq. (5.29) as generators.

Transformations of SO(4) to preserve also ξ_4 constitute a subgroup isomorphic to SO(3), and we denote it simply SO(3). Its matrices have the form

$$C = \left[\begin{array}{c|c} c_{\alpha\beta} & 0 \\ \hline 0 & 1 \end{array}\right] \tag{5.35}$$

where $(o_{\alpha\beta})(1 \le \alpha, \beta \le 3)$ is an orthogonal matrix of the third order with determinant 1, and **1** in the lower right corner is the unit matrix of the third order. Generators of the Lie algebra of SO(3) subgroup are $L_{\alpha\beta}(1 \le \alpha, \beta \le 3)$ or their independent linear combination $J_k + K_k$ $(k = 1, 2, 3)$.

So we have described in detail the construction of the chain of groups (eq. (1.82)).

As is readily verified using eq. (5.31), generators J_k $(k = 1, 2, 3)$ form a Lie subalgebra with the same commutation relations as those of SO(3); hence, the matrices $O_J = e^{-i(\alpha_1 J_1 + \alpha_2 J_2 + \alpha_3 J_3)}$ constitute a subgroup of SO(4) isomorphic to SO(3). Denote this subgroup $\mathrm{SO}(3)_J$. Similarly, generators $K_k (k = 1, 2, 3)$ generate a subgroup of matrices $O_K = e^{-i(\alpha_1 K_1 + \alpha_2 K_2 + \alpha_3 K_3)}$ isomorphic to SO(3) which we denote $\mathrm{SO}(3)_K$. From eq. (5.31), we have $[J_k, K_l] = 0 (k, l = 1, 2, 3)$ and the exponential expansion shows that O_J commutes with O_K.

Writing the rotation matrices of the fourth order $O^{(4)}$ in the form $e^{-iA} = e^{-iA_J} e^{-iA_K}$, where $A_J = \sum_{k=1}^{3} \alpha_k J_k, A_K = \sum_{l=1}^{3} \beta_l K_l$, one can verify that matrices sufficiently close to unity are uniquely represented as products of commuting matrices from subgroups $\mathrm{SO}(3)_J$ and $\mathrm{SO}(3)_K$, respectively, and also close to the unity matrix. This is expressed by the following definition: group SO(4) is locally a direct product of the two above subgroups:[45]

45 Note that *in the large* (i.e. without assuming all matrices to be near unity), the decomposition (eq. (5.36)) is not unique, because the correspondence between the elements of a Lie group and its Lie algebra need to be a one-to-one correspondence. Even the local expansion (eq. (5.36)) is, in some sense, exceptional: SO(4) is the only SO(n) group which can be expanded this way.

$$SO(4) = SO(3)_J \times SO(3)_K \tag{5.36}$$

5.3 A special representation of the conformal group

We need a special representation of the group SO(4,2). To construct it, we begin with representations of the subgroups SO(4). The procedure is facilitated by the expansion (5.36); further, we will consider only *local* representations, so that the local nature of this expansion will not be an obstacle to use it.

All irreducible representations of SO(4) can be constructed by means of eq. (5.36) (see Appendix B). Denote $SO(3)_J$, $SO(3)_K$ the subgroups of SO(4) with generators $J_k, K_k (k = 1, 2, 3)$, respectively. Then every irreducible representation T of group SO(4) has the following structure. Space R of the representation T is a tensor product of spaces $\mathsf{R}_1, \mathsf{R}_2$ with irreducible representations D_{j1}, corr. D_{j2} of the subgroups $SO(3)_J$, corr. $SO(3)_K$ having dimensions $2j_1 + 1$, corr. $2j_2 + 1$, so that the dimension T is $2j_1 + 1, 2j_2 + 1$ (j_1, j_2 are integral or half-integral numbers). The representation T is constructed from D_{j_1}, D_{j_2} according to eq. (3.141) with the bases $|\sigma\rangle$, corr. $|\tau\rangle$ consisting of eigenvectors of the operator $J_3 K_3 (\sigma = -j_1, -j_1 + 1, ..., j_1 - 1, j_1; \tau = -j_2, -j_2 + 1, ..., j_2 - 1, j_2)$. Action of generators J_k, K_k upon the basis vectors $|\sigma, \tau\rangle$ is given by

$$\begin{aligned}
J_+|\sigma,\tau\rangle &= [(j_1 + \sigma + 1)(j_1 - \sigma)]^{1/2}|\sigma + 1, \tau\rangle \\
J_-|\sigma,\tau\rangle &= [(j_1 + \sigma)(j_1 - \sigma + 1)]^{1/2}|\sigma - 1, \tau\rangle \\
J_3|\sigma,\tau\rangle &= \sigma|\sigma,\tau\rangle \\
K_+|\sigma,\tau\rangle &= [(j_2 + \tau + 1)(j_2 - \tau)]^{1/2}|\sigma, \tau + 1\rangle \\
K_-|\sigma,\tau\rangle &= [(j_2 + \tau)(j_2 - \tau + 1)]^{1/2}|\sigma, \tau - 1\rangle \\
K_3|\sigma,\tau\rangle &= \tau|\sigma,\tau\rangle
\end{aligned} \tag{5.37}$$

(where vector $|\sigma, \tau\rangle$ is replaced by zero for $\sigma > j_1, \tau > j_2$ or $\sigma < -j_1, \tau < -j_2$). The described representation of SO(4), denoted $D_{j_1 j_2}$, is irreducible and unitary (see Appendix B, Section 2).

Since factors $SO(3)_J$, $SO(3)_K$ are isomorphic, obtain local representation of SO(3) as a tensor product $D_{j_1} \otimes D_{j_2}$ (see eq. (3.146)) from the constructed representation of their local product $SO(4) = SO(3)_J \times SO(3)_K$. As follows from eq. (3.152), generators of SO(3) are represented by operators $J_k + K_k$. But the same representation is true for the generators of SO(3) to preserve ξ_4. Thus, the reduction of $D_{j_1 j_2}$ onto this subgroup results in its representation $D_{j_1} \otimes D_{j_2}$. The latter is, by Clebsch-Gordan theorem, decomposed into a sum of irreducible representations SO(3) of dimensions $2j + 1$, where $j = |j_1 - j_2|, |j_1 - j_2| + 1, ..., j_1 + j_2$.

Now describe the structure of Fock representation of group SO(4) introduced in Chapter 1 (see eq. (1.71)). Denote the space of the representation Φ, and its irreducible

subspaces defined in spaces F_n denote Φ_n (see eqs. (1.72) and (1.33)). Then (see Appendix B), the irreducible representation Φ_n decomposes into the sum of irreducible representations of the subgroup SO(3) of dimensions 1, 3, …, $2n-1$ (see eqs. (1.73) and (1.34)). In view of the above-described structure of irreducible representations of the group SO(4), the smallest dimension 1 is $2|j_1 - j_2| + 1$, whence $j_1 = j_2$; so the representation Φ_n has the form $D_{j_1 j_2}$. Since the highest dimension is $2n - 1 = 2(j_1 + j_2) + 1 = 4j + 1$, we have $j = \frac{n-1}{2}$ and

$$\Phi = \Phi_1 \oplus \Phi_2 \oplus \ldots \oplus \Phi_n \oplus \ldots, \text{ where } \Phi_n = D_{\frac{n-1}{2},\frac{n-1}{2}} \tag{5.38}$$

Thus each subspace F_n has an orthonormal basis $|\sigma, \tau\rangle$ which we denote $|j, \sigma, \tau\rangle \left(j = \frac{n-1}{2}\right)$. All these bases constitute an orthonormal basis of the Fock space F:

$$|j, \sigma, \tau\rangle \left(j = 0, 1/2, 1, 3/2, \ldots; \sigma = -j, -j+1, \ldots, j-1, j; \tau = -j, -j+1, \ldots, j-1, j \right) \tag{5.39}$$

where the Lie algebra of SO(4) acts according to eq. (5.37) with $j_1 = j_2 = j$.

With basis (5.39), the Fock representation of SO(4) will be extended to a unitary representation of the conformal group SO(4,2) *in the same space* F. To do that, the method described in Section 3.3 will be used: generators of group SO(4) correspond to Hermitian operators acting in space F with the same commutation relations. It is more convenient to use linear combinations of generators with complex coefficients $J_\pm$, J_3, … (see eq. (5.31)) rather than generators as such, making sure that operators corresponding to J_1, J_2, J_3, … be Hermitian. Operators will be denoted with the same letters as the generators of the Lie algebra they represent. Then the desired operators are defined as follows:

$$\begin{aligned}
J_+|j, \sigma, \tau\rangle &= [(j+\sigma+1)(j-\sigma)]^{1/2}|j, \sigma+1, \tau\rangle \\
J_-|j, \sigma, \tau\rangle &= [(j+\sigma)(j-\sigma+1)]^{1/2}|j, \sigma-1, \tau\rangle \\
J_3|j, \sigma, \tau\rangle &= \sigma|j, \sigma, \tau\rangle
\end{aligned}$$

$$\begin{aligned}
K_+|j, \sigma, \tau\rangle &= [(j+\tau+1)(j-\tau)]^{1/2}|j, \sigma, \tau+1\rangle \\
K_-|j, \sigma, \tau\rangle &= [(j+\tau)(j-\tau+1)]^{1/2}|j, \sigma, \tau-1\rangle \\
K_3|j, \sigma, \tau\rangle &= \tau|j, \sigma, \tau\rangle
\end{aligned}$$

$$\begin{aligned}
P_+|j, \sigma, \tau\rangle &= i[(j+\sigma+1)(j-\tau+1)]^{1/2}\left|j+\frac{1}{2}, \sigma+\frac{1}{2}, \tau-\frac{1}{2}\right\rangle \\
P_-|j, \sigma, \tau\rangle &= -i[(j+\sigma)(j-\tau)]^{1/2}\left|j-\frac{1}{2}, \sigma-\frac{1}{2}, \tau+\frac{1}{2}\right\rangle \\
P_0|j, \sigma, \tau\rangle &= \left(j+\frac{\sigma-\tau+1}{2}\right)|j, \sigma, \tau\rangle
\end{aligned}$$

$$
\begin{aligned}
Q_+|j,\sigma,\tau\rangle &= -i[(j-\sigma+1)(j+\tau+1)]^{1/2}\left|j+\frac{1}{2},\sigma-\frac{1}{2},\tau+\frac{1}{2}\right\rangle\\
Q_-|j,\sigma,\tau\rangle &= i[(j-\sigma)(j+\tau)]^{1/2}\left|j-\frac{1}{2},\sigma+\frac{1}{2},\tau-\frac{1}{2}\right\rangle\\
Q_0|j,\sigma,\tau\rangle &= \left(j-\frac{\sigma-\tau-1}{2}\right)|j,\sigma,\tau\rangle\\
S_+|j,\sigma,\tau\rangle &= -i[(j+\sigma+1)(j+\tau+1)]^{1/2}\left|j+\frac{1}{2},\sigma+\frac{1}{2},\tau+\frac{1}{2}\right\rangle\\
S_-|j,\sigma,\tau\rangle &= i[(j+\sigma)(j+\tau)]^{1/2}\left|j-\frac{1}{2},\sigma-\frac{1}{2},\tau-\frac{1}{2}\right\rangle\\
S_0|j,\sigma,\tau\rangle &= \left(j+\frac{\sigma+\tau+1}{2}\right)|j,\sigma,\tau\rangle\\
T_+|j,\sigma,\tau\rangle &= i[(j-\sigma+1)(j-\tau+1)]^{1/2}\left|j+\frac{1}{2},\sigma-\frac{1}{2},\tau-\frac{1}{2}\right\rangle\\
T_-|j,\sigma,\tau\rangle &= -i[(j-\sigma)(j-\tau)]^{1/2}\left|j-\frac{1}{2},\sigma+\frac{1}{2},\tau+\frac{1}{2}\right\rangle\\
T_0|j,\sigma,\tau\rangle &= \left(j-\frac{\sigma+\tau-1}{2}\right)|j,\sigma,\tau\rangle
\end{aligned}
\tag{5.40}
$$

where symbols $|j,\sigma,\tau\rangle$ on the right not satisfying the conditions $-j\le\sigma\le j$, $-j\le\tau\le j$ are assumed to be replaced by zeros.

Commutation relations for these operators are readily verified. For example, find $[Q_+,S_-]$. According to eq. (5.40),

$$
S_-|j,\sigma,\tau\rangle = i[(j+\sigma)(j+\tau)]^{1/2}\left|j-\frac{1}{2},\sigma-\frac{1}{2},\tau-\frac{1}{2}\right\rangle. \tag{5.41}
$$

Apply to both sides of eq. (5.41) the operator Q_+; using eq. (5.40), but substituting j by $j-\frac{1}{2}$, σ by $\sigma-\frac{1}{2}$, τ by $\tau-\frac{1}{2}$, we have

$$
Q_+S_-|j,\sigma,\tau\rangle = (-i)i[(j+\sigma)(j+\tau)]^{1/2}[(j-\sigma+1)(j+\tau)]^{1/2}|j,\sigma-1,\tau\rangle \tag{5.42}
$$

Similarly,

$$
\begin{aligned}
Q_+|j,\sigma,\tau\rangle &= -i[(j-\sigma+1)(j+\tau+1)]^{1/2}\left|j+\frac{1}{2},\sigma-\frac{1}{2},\tau+\frac{1}{2}\right\rangle,\\
S_-Q_+|j,\sigma,\tau\rangle &= i(-i)[(j-\sigma+1)(j+\tau+1)]^{1/2}[(j+\sigma)(j+\tau+1)]^{1/2}|j,\sigma-1,\tau\rangle,
\end{aligned}
\tag{5.43}
$$

Using again eq. (5.41), we get

$$
\begin{aligned}
[Q_+S_-]|j,\sigma,\tau\rangle &= [(j+\tau)\sqrt{(j+\sigma)(j-\sigma+1)}-(j+\tau+1)\sqrt{(j+\sigma)(j-\sigma+1)}\,]|j,\sigma-1,\tau\rangle\\
&= -\sqrt{(j+\sigma)(j-\sigma+1)}\,|j,\sigma-1,\tau\rangle = -J_-|j,\sigma,\tau\rangle
\end{aligned}
\tag{5.44}
$$

As $[Q_+S_-]$ and J_- take equal values for all basis vectors, they coincide; therefore, for the operators Q_+, S_-, J_-, the following commutation relation is true:

$$[Q_+S_-] = -J_- \tag{5.45}$$

But from eq.(5.32), it follows that the same relation is true for the matrices of the sixth order denoted by the same letters. All other relations of eq. (5.32) are verified in the same way.

Verify now that operator P is Hermitian (the verification for all the other operators $J_k, K_k, P_k, Q_k, S_k, T_k$ is similar). By definition of $P_\pm$, we have $P_2 = \frac{1}{2i}(P_+ - P_-)$ and from eq. (5.40),

$$\begin{aligned} P_2|j,\sigma,\tau\rangle = -\frac{1}{2}i\Big\{ & i[(j+\sigma+1)(j-\tau+1)]^{1/2}\left|j+\frac{1}{2},\sigma+\frac{1}{2},\tau-\frac{1}{2}\right\rangle \\ & -(-i)[(j+\sigma)(j-\tau)]^{1/2}\left|j-\frac{1}{2},\sigma-\frac{1}{2},\tau+\frac{1}{2}\right\rangle\Big\} \end{aligned} \tag{5.46}$$

Since the basis is orthonormal, the matrix elements of P_2 are

$$\begin{aligned} \langle j',\sigma',\tau'|P_2 \mid j,\sigma,\tau\rangle = \frac{1}{2}\Big\{ & [(j+\sigma+1)(j-\tau+1)]^{1/2}\delta_{j',j+\frac{1}{2}}\delta_{\sigma',\sigma+\frac{1}{2}}\delta_{\tau',\tau-\frac{1}{2}} \\ & +[(j+\sigma)(j-\tau)]^{1/2}\delta_{j',j-\frac{1}{2}}\delta_{\sigma',\sigma-\frac{1}{2}}\delta_{\tau',\tau+\frac{1}{2}}\Big\} \end{aligned} \tag{5.47}$$

where $\delta_{\alpha\beta} = 0$ for $\alpha \neq \beta$, $\delta_{\alpha\beta} = 1$ for $\alpha = \beta, \alpha, \beta$ integral or half-integral. There are only two nonzero matrix elements:

$$\left\langle j+\frac{1}{2},\sigma+\frac{1}{2},\tau-\frac{1}{2}|P_2|\ j,\sigma,\tau\right\rangle = \frac{1}{2}[(j+\sigma+1)(j-\tau+1)]^{1/2} \tag{5.48}$$

$$\left\langle j-\frac{1}{2},\sigma-\frac{1}{2},\tau+\frac{1}{2}|P_2|\ j,\sigma,\tau\right\rangle = \frac{1}{2}[(j+\sigma)(j-\tau)]^{1/2} \tag{5.49}$$

Find the element symmetric to eq. (5.48) relative to the main diagonal. To do that, rearrange in eq. (5.48), the vectors $|j+\frac{1}{2},\sigma+\frac{1}{2},\tau-\frac{1}{2}\rangle$ and $|j,\sigma,\tau\rangle$ and use eq. (5.49) to calculate the resulting element:

$$\begin{aligned} \left\langle j,\sigma,\tau|P_2|\ j+\frac{1}{2},\sigma+\frac{1}{2},\tau-\frac{1}{2}\right\rangle &= \frac{1}{2}\left\{\left[\left(j+\frac{1}{2}\right)+\left(\sigma+\frac{1}{2}\right)\right]\left[\left(j+\frac{1}{2}\right)-\left(\tau-\frac{1}{2}\right)\right]\right\}^{1/2} \\ &= \frac{1}{2}[(j+\sigma+1)(j-\tau+1)]^{1/2} \end{aligned} \tag{5.50}$$

which coincides with eq. (5.48). Thus, matrix P_2 is Hermitian, and it follows, like for the operators in a finite-dimensional space,

$$\langle\Psi|P_2|X\rangle = \langle X|P_2|\Psi\rangle^* \tag{5.51}$$

for any vectors Ψ, X of the space F.

Thus, *eq.* (5.40) *define a unitary representation of the group* SO(4,2) *in the Fock space.*[46] Denote this representation $\{T_C\}$. Note that eq. (5.40) includes relations for J_k, K_k to define representations Φ_n in the subspaces F_n (see eq. (5.37) for $j_1 = j_2 = j$) and, therefore, Fock representation Φ on the subgroup SO(4). Thus, we have actually obtained the *expansion* of Fock representation on the conformal group.

Now we show that representation $\{T_C\}$ is *irreducible*. Since subspaces F_n are irreducible even for subgroups SO(4), it is sufficient to prove that the operators of Lie algebra of SO(4,2) connect all these subspaces with each other; then the space F is irreducible for the Lie algebra, and, therefore, for the group SO(4,2). Since the operators of the Lie algebra are linear combinations of those of its complex envelope, it is sufficient to prove that the operators $P_\pm, Q_\pm, S_\pm, T_\pm$ connect these subspaces. It suffices to consider the operators

$$\Gamma_+ = P_+ + Q_+, \Gamma_- = P_- + Q_- \tag{5.52}$$

From eq. (5.40), it follows that

$$\begin{aligned}\Gamma_+|j,\sigma,\tau\rangle = {} & i[(j+\sigma+1)(j-\tau+1)]^{1/2}\left|j+\frac{1}{2},\sigma+\frac{1}{2},\tau-\frac{1}{2}\right\rangle \\ & - i[(j-\sigma+1)(j+\tau+1)]^{1/2}\left|j+\frac{1}{2},\sigma-\frac{1}{2},\tau+\frac{1}{2}\right\rangle\end{aligned} \tag{5.53}$$

$$\begin{aligned}\Gamma_-|j,\sigma,\tau\rangle = {} & -i[(j+\sigma)(j-\tau)]^{1/2}\left|j-\frac{1}{2},\sigma-\frac{1}{2},\tau+\frac{1}{2}\right\rangle \\ & + i[(j-\sigma)(j+\tau)]^{1/2}\left|j-\frac{1}{2},\sigma+\frac{1}{2},\tau-\frac{1}{2}\right\rangle\end{aligned} \tag{5.54}$$

As Γ_+ increases j by $\frac{1}{2}$, that is, n by 1, eq. (5.53) means that Γ_+ carries F_n into F_{n+1}, and similarly Γ_- carries F_n into F_{n-1}. Now we show that the right side of eq. (5.53) is always nonzero. Since $-j \le \sigma \le j$, $-j \le \tau \le j$, we have $-(j+\frac{1}{2}) \le \sigma \pm \frac{1}{2} \le j+\frac{1}{2}$, $-(j+\frac{1}{2}) \le \tau \pm \frac{1}{2} \le j+\frac{1}{2}$, so that both vectors on the right side of eq. (5.53) are nonzero and orthogonal, and having nonzero coefficients which proves the statement. For Γ_-, it is sufficient to show that for $n \ge 2$, the vector $|j, \frac{1}{2}, 0\rangle$ is carried into a nonzero vector; but in this case, the right side of eq. (5.54) reduces to the nonzero first term.

As it will be shown below, operators Γ_+, Γ_- are used to describe Mendeleevian homologous series.

Basis vectors Ψ_{nlm} of space F (Table 5.1) do not coincide with the vectors of basis $|j,\sigma,\tau\rangle$: they are eigenvectors of $L_{12} = J_3 + K_3$ and $L^2 = L_{12}^2 + L_{23}^2 + L_{31}^2$ (which belong to

46 Of course, eq. (5.3.4) is derived with general methods of the theory of representations (se, e.g. Yao, 1967), which make it possible to find *all* unitary representations of the conformal group. Here we verify the equations only in the case we are interested in now. In Yao (1967) (p. II, p. 1625), this representation is denoted E^+.

eigenvalues m and $l(l+1)$, respectively) rather than eigenvectors of J_3, K_3. The operator $J_3 + K_3$ belongs to Lie algebra of subgroup SO(3), whereas L^2 is the Casimir operator of this subgroup and belongs to its universal enveloping algebra. The basis Ψ_{nlm} is important from the physical viewpoint while vectors $|j, \sigma, \tau\rangle$ are good to construct representations, as they are associated with the direct decomposition (eq. (5.36)) of SO(4) group.

Note also that the operator $-L_{56} = P_0 + Q_0 = S_0 + T_0$, which we denote R_0, commutes with subgroup SO(4)and, therefore, it is its Casimir operator; this is readily seen from eq. (5.25). This operator belongs to the Lie algebra of SO(4,2) (but not of its subgroup SO(4)). The value of R_0 on the space F_n is easily found by applying the operator to any vector $|j, \sigma, \tau\rangle$ and using eq. (5.40) for P_0, Q_0 or S_0, T_0; this value is n. Thus, the vector Ψ_{nlm} can be described as the common eigenvector of operators $R_0, L^2, J_3 + K_3$ with eigenvalues $n, l(l+1), m$, respectively. Thus, the numbers *n, l, m* are characterized as the *quantum numbers of the conformal group*. As already mentioned, number l has no direct group-theoretical meaning and is used only to obtain $l(l+1)$, but is also often called a *quantum number*. The ranges of quantum numbers for the representation $\{T_C\}$ are indicated in eq. (5.1).

5.4 The symmetry group of the system of elements

By comparing Table 5.1 with Table 1.1 to image the basis of the representation of the conformal group $\{T_C\}$, easily see that quantum numbers of the conformal group *n, l, m* do not provide a one-to-one numeration for the elements: the fourth Madelung number *s* has no group-theoretical interpretation. Compared with Table 1.1, the system of elements "redoubles" like it happens with spin splitting of the hydrogen energy levels. Just as each set of quantum numbers (*n, l, m*) corresponds to *two* hydrogen energy levels with different values of "spin projection" *s*, each set (*n, l, m*) is associated with *two* elements associated with different Madelung numbers *s*. This suggests the idea to introduce a "chemical spin," that is, to use Pauli's mathematical approach and use two-component wave-functions rather than one-component wave-functions. There is, of course, an essential difference between these two systems: whereas the splitting of energy levels of hydrogen is small as compared to the energy differences corresponding to different sets *n, l, m*, the elements with the same values of *n, l, m* and different *s* differ in their atomic weights (and other properties) as much as elements with different *n, l, m*. However, as we saw in the unitary symmetry of hadrons, great variation of masses in the multiplets is not an obstacle to describe them with symmetry groups. So we will use the spin apparatus and neglect the quantitative difference between the above systems.

We defined the representation $\{T_C\}$ of the group SO(4,2) in the Fock space F, consisting of functions $\Psi(\xi_1, \xi_2, \xi_3, \xi_4)$ of four variables defined on the sphere $S^3(\xi_1^2 + \xi_2^2 + \xi_3^2 + \xi_4^2 = 1)$ of the four-dimensional Euclidean space R^4. Functions Ψ will further play a role similar to one-component Schrödinger wave functions $\psi(x, y, z)$.

Introduce *two-component* functions similar to a two-component wave functions Pauli (see eq. (4.1)):

$$\Theta = \begin{bmatrix} \Psi_1(\xi_1, \xi_2, \xi_3, \xi_4) \\ \Psi_2(\xi_1, \xi_2, \xi_3, \xi_4) \end{bmatrix} \tag{5.55}$$

where Ψ_1, Ψ_2 are functions defined on S^3, independent of each other and having finite integrals over the sphere:

$$\int_{S^3} |\Psi_\sigma|^2 d\Omega < \infty (\sigma = 1, 2) \tag{5.56}$$

Introduce in the space of two-component functions Θ a scalar product (see eqs. (1.49) and (4.3)): for

$$\Theta = \begin{bmatrix} \Psi_1(\xi_1, \xi_2, \xi_3, \xi_4) \\ \Psi_2(\xi_1, \xi_2, \xi_3, \xi_4) \end{bmatrix}, \quad T = \begin{bmatrix} \Phi_1(\xi_1, \xi_2, \xi_3, \xi_4) \\ \Phi_2(\xi_1, \xi_2, \xi_3, \xi_4) \end{bmatrix} \tag{5.57}$$

define

$$\langle T|\Theta\rangle = \frac{1}{2\pi^2}\int_{S^3} (\Phi_1^*\Psi_1 + \Phi_2^*\Psi_2) d\Omega = \langle \Phi_1|\Psi_1\rangle + \langle \Phi_2|\Psi_2\rangle \tag{5.58}$$

(where scalar product on the right are taken in space F). Thus, the two-component functions constitute a Hilbert space, which we denote F^2.

Now define an action of group SU(2) × SO(4,2) in the space F^2. We will not follow eq. (4.7), where the same rotation group SO(3) simultaneously acts for wave functions ψ_τ and transforms the components using matrix $(u_{\sigma\tau})$.This construction corresponds the so-called "strong spin–orbit coupling." In our case *different* groups will be used to transform functions Ψ_σ and to obtain linear transformations of the components of Θ. This construction is similar to "weak spin–orbit coupling." The group to act on space F^2 will be

$$\mathrm{SU}(2) \times \mathrm{SO}(4, 2) \tag{5.59}$$

Elements of o group (eq. (5.59)) are pairs (u, C), where u is a matrix of SU(2) and C is a matrix of SO(4,2) (see Section 3.5); the multiplication of such pairs is given by

$$(u_1, C_1)(u_2, C_2) = (u_1u_2, C_1C_2) \tag{5.60}$$

Now define representation $\{T_{u,C}\}$ of group SU(2) × SO(4,2) in the space of two-component functions F^2 by the rule described in Section 3.5. Construct a space $C^2 \otimes \mathsf{F}$, where C^2 is a two-dimensional complex space with basis e_1, e_2. The vectors of this space can be represented as

$$e_1 \otimes \Psi_1(\xi_1, \xi_2, \xi_3, \xi_4) + e_2 \otimes \Psi_2(\xi_1, \xi_2, \xi_3, \xi_4) \tag{5.61}$$

Then action of an element (u, C) of the group SU(2) × SO(4,2) on the vector (5.61), as defined in eq. (3.141), produces the vector

$$\begin{aligned} T_u e_1 \otimes T_C \Psi_1 + T_u e_2 \otimes T_C \Psi_2 &= (u_{11} e_1 + u_{21} e_2) \otimes T_C \Psi_1 + (u_{12} e_1 + u_{22} e_2) \otimes T_C \Psi_2 \\ &= e_1 \otimes (u_{11} T_C \Psi_1 + u_{12} T_C \Psi_2) + e_2 \otimes (u_{21} T_C \Psi_1 + u_{22} T_C \Psi_2) \end{aligned} \tag{5.62}$$

Writing the vector (5.61) as a two-component function,

$$\Theta = \begin{bmatrix} \Psi_1(\xi_1, \dots, \xi_4) \\ \Psi_2(\xi_1, \dots, \xi_4) \end{bmatrix} \tag{5.63}$$

and, similarly, vector (5.62) as

$$\Theta' = \begin{bmatrix} \Psi'_1(\xi_1, \dots, \xi_4) \\ \Psi'_2(\xi_1, \dots, \xi_4) \end{bmatrix} \tag{5.64}$$

obtain

$$T_{u,C}\ \Theta = \Theta' \tag{5.65}$$

where

$$u = (u_{\sigma\tau}), \Psi'_\sigma = \sum_{\tau=1}^{2} u_{\sigma\tau} T_C(\Psi_\tau). \tag{5.66}$$

This means that components Ψ_τ are first transformed by operator T_C corresponding to the matrix C, as defined above, and then the resulting functions are linearly transformed by matrix u.

Now show that eq. (5.66) defines a representation. If $u = u_1 u_2$, $C = C_1 C_2$, then

$$T_{u_2,C_2}(\Theta) = \Theta', \quad T_{u_1,C_1}(\Theta') = \Theta'', \tag{5.67}$$

where

$$\begin{aligned} \Psi'_\rho &= \sum_{\tau=1}^{2} (u_2)_{\rho\tau} T_{C_2}(\Psi_\tau) \\ \Psi''_\sigma &= \sum_{\rho=1}^{2} (u_1)_{\sigma\rho} T_{C_1}(\Psi'_\rho) = \sum_{\rho,\tau=1}^{2} (u_1)_{\sigma\rho} (u_2)_{\rho\tau} T_{C_1} T_{C_2}(\Psi_\tau) \\ &= \sum_{\tau=1}^{2} (u_1 u_2)_{\sigma\tau} T_{C_1 C_2}(\Psi_\tau) = \sum_{\tau=1}^{2} u_{\sigma\tau} T_C(\Psi_\tau) \end{aligned} \tag{5.68}$$

and hence Θ" = $T_{u,C}$(Θ).

Show that the representation $\{T_{u,C}\}$ is unitary. Let $\Theta = \begin{bmatrix} \Psi_1 \\ \Psi_2 \end{bmatrix}$, $Z = \begin{bmatrix} \Phi_1 \\ \Phi_2 \end{bmatrix}$. Since matrix u and representation T_C are unitary, we have

$$\begin{aligned}\langle\Theta'|Z'\rangle &= \frac{1}{2\pi^2}\int_{S^3}\sum_{\sigma=1}^{2}\Psi'^{*}_{\sigma}\Phi'_{\sigma}d\Omega = \frac{1}{2\pi^2}\int_{S^3}\sum_{\sigma,\tau,\rho=1}^{2}u^{*}_{\sigma\tau}T_C(\Psi_\tau)^{*}u_{\sigma\rho}T_C(\Phi_\rho)d\Omega\\ &= \frac{1}{2\pi^2}\int_{S^3}\sum_{\tau,\rho=1}^{2}\left(\sum_{\sigma=1}^{2}u^{*}_{\sigma\tau}u_{\sigma\rho}\right)T_C(\Psi_\tau)^{*}T_C(\Phi_\rho)d\Omega\\ &= \frac{1}{2\pi^2}\int_{S^3}\sum_{\tau,\rho=1}^{2}\delta_{\tau\rho}T_C(\Psi_\tau)^{*}T_C(\Phi_\rho)d\Omega = \sum_{\tau=1}^{2}\frac{1}{2\pi^2}\int_{S^3}T_C(\Psi_\tau)^{*}T_C(\Phi_\tau)d\Omega\\ &= \sum_{\tau=1}^{2}\frac{1}{2\pi^2}\int_{S^3}\Psi^{*}_{\tau}\Phi_\tau d\Omega = \langle\Theta|Z\rangle\end{aligned} \tag{5.69}$$

Show that representation $\{T_{u,C}\}$ is irreducible. Let F be an invariant subspace of F^2, $\Theta = \begin{bmatrix}\Psi_1\\ \Psi_2\end{bmatrix}$ is a vector in $\widetilde{\mathsf{F}}$. Then operator $T_{\sigma_3,1}$ of the Lie algebra (σ_3 is a Pauli matrix and 1 is a sixth-order unit matrix) carries Θ into vector $\Theta' = \begin{bmatrix}\Psi_1\\ -\Psi_2\end{bmatrix}$ also belonging to $\widetilde{\mathsf{F}}$; but $\begin{bmatrix}2\Psi_1\\ 0\end{bmatrix} = \Theta + \Theta'$ also belongs to $\widetilde{\mathsf{F}}$. Applying to this vector operators $T_{1,C}$ and from irreducibility of $\{T_C\}$ obtain that *all* vectors of the form $\begin{bmatrix}\Psi\\ 0\end{bmatrix}$ and, similarly, $\begin{bmatrix}0\\ \Psi_2\end{bmatrix}$ belong to $\widetilde{\mathsf{F}}$. But the sums of such vectors constitute F_2, so $\widetilde{\mathsf{F}} = \mathsf{F}_2$.

Thus, an irreducible unitary representation $\{T_{u,C}\}$ of group SU(2) × SO(4,2) in the space of two-component functions Θ has been constructed. To simplify notations, denote henceforward operators $T_{u,1}$ by u, the operators $T_{1,C}$ by C, and do the same with the operators of the Lie algebra. Then n, l, m still remain quantum numbers of the group corresponding to operators $R_0, L^2, J_3 + K_3$; the eigenvectors of these operators $\Theta = \begin{bmatrix}\Psi_1\\ \Psi_2\end{bmatrix}$ have components which are eigen functions of corresponding operators of group SO(4,2). All these operators act on each component Θ separately. On the other hand, operator $\tau_3 = \frac{1}{2}\sigma_3$ from the Lie algebra of subgroup SU(2) × 1, carries vector $\Theta = \begin{bmatrix}\Psi_1\\ \Psi_2\end{bmatrix}$ into $\Theta' = \begin{bmatrix}\Psi_1\\ -\Psi_2\end{bmatrix}$. The eigenvalues of this operator are $s = \pm\,{}^1\!/_2$, and corresponding eigenvectors have the form $\begin{bmatrix}\Psi\\ 0\end{bmatrix}$ and $\begin{bmatrix}0\\ \Psi\end{bmatrix}$. Thus, *the Madelung number s is a quantum number of the group* SU(2) × SO(4,2). Operator τ_3 commutes with all operators of the subgroup 1 × SO(4,2), and therefore with its Lie algebra. Therefore, operators $R_0, L^2, J_3 + K_3, \tau_3$ commute with each other. Their common eigenvectors are

$$\left|n, l, m, \frac{1}{2}\right\rangle = \begin{bmatrix}\Psi_{nlm}\\ 0\end{bmatrix}, \left|n, l, m, -\frac{1}{2}\right\rangle = \begin{bmatrix}0\\ \Psi_{nlm}\end{bmatrix} \tag{5.70}$$

with eigenvalues, $n, l(l+1), m, \frac{1}{2}$ И $n, l(l+1), m, -\frac{1}{2}$, respectively.

From eq. (3.129), we have

$$\tau_+\left|n,l,m,-\frac{1}{2}\right\rangle = \left|n,l,m,\frac{1}{2}\right\rangle, \tau_-\left|n,l,m,\frac{1}{2}\right\rangle = \left|n,l,m,-\frac{1}{2}\right\rangle,$$
$$\tau_3|n,l,m,\sigma\rangle = \sigma|n,l,m,\sigma\rangle\left(\sigma = -\frac{1}{2},\frac{1}{2}\right) \tag{5.71}$$

whereas the operators of the Lie algebra of SO(4,2) act only on the numbers n, l, m, but not on s. The basis $|n,l,m,s\rangle$ is in am one-to-one correspondence with chemical elements as suggested by the Madelung numeration (Table 5.1). Since empirical numbering Madelung provides good ordering of elements according to their properties (see Section 1), and the Madelung number are quantum numbers of group SU(2) × SO(4,2), this group is reasonably assumed related to the symmetry of the system of elements.

Now return to the numeration of Madelung. At the first acquaintance with Table 5.1, we simply noted that some regularities are revealed if the table is filled with symbols in a certain order, for example, change of a single number n results in Mendeleevian homologous series to occupy horizontal rows of the table. Obviously, there is a relationship between an element and its "address" in the table, that is, the set of numbers (n, l, m, s). To find the relationship, the elements are to be denoted. From a group-theoretical viewpoint, the elements are naturally denoted by the sets of their quantum numbers; but since our goal is a correspondence with the traditional description, we will represent them by their atomic numbers which have a direct experimental meaning. Note that atomic number is not a quantum number, neither a part of our theory, and serves only as an experimental characteristic of an element to introduce it into the group description. So, it is necessary to establish a one–one correspondence between positive integers $Z = 1, 2, 3, \ldots$ and a set of numbers (n, l, m, s) satisfying condition (5.1):

$$Z \leftrightarrow (n,l,m,s) \tag{5.72}$$

This correspondence is given by the "Madelung lexicographic rule":

1) The elements are arranged in order of increasing atomic number Z.
2) The sets (n, l, m, s) are arranged in order of increasing $n + l$; for fixed $n + l$, in order of increasing n; for fixed $n + l$, n, in order of increasing m; for fixed $n + l$, n, m, in order of increasing s.
3) Z-th element corresponds to the Z-th set.

Evidently, the elements of Table 5.1 satisfy this rule. Note again that the Madelung rule is not a part of our present theory but only a way to connect it with the experiment. Therefore, it is not the rule (5.72) itself which is to be justified, but the choice of parameters n, l, m, s obeying rule (5.1) and serving to numerate the elements; the justification is that these parameters are quantum numbers of group SU(2) × SO(4,2)

and that group-theoretical approach allows classification of the elements according to their properties.

First of all, group interpretation shows that Madelung numeration is not very natural and needs to be changed. In fact, "lexicographic rule" includes the *sum* $n + l$ together with n, m, s rather than numbers n, l, m, s as such. As mentioned above, l by itself is not a *genuine* quantum number, that is, an eigenvalue of some operator from the universal enveloping algebra of group SU(2) × SO(4,2); such quantum number is $l(l + 1)$ which is the eigenvalue of operator $L^2 = L_{12}^2 + L_{23}^2 + L_{31}^2$, whereas l merely *labels* this quantum number.

In this sense, l is sometimes called a quantum number. This means that the sum $n + l$ has no group-theoretical meaning: it is a sum of a genuine quantum number n (eigenvalue of the operator $R_0 = -L_{56}$) and number l (which is not a quantum number). Therefore, from the group-theoretical viewpoint, number $n + l$ cannot be part of the "lexicographic rule." Therefore, Madelung numeration is to be replaced by another numeration which would describe the regularities of element properties and would be free of the above defect.

If Table 5.1 is watched "along the diagonal," value $n + l$ is found to be constant for the rectangles on the diagonals. Consider all rectangles with odd values of $n + l$ and define for them $v = \frac{1}{2}(n + l + 1)$. For $v = 1$, we obtain the rectangle (*H*, *He*); for $v = 2$, a series of rectangles (Na,Mg),(B–Ne); for $v = 3$, a series of rectangles (Rb,Sr),(Ga – Kr),(Sc – Zn); and so on. For rectangles with even values, $n + l$ define $v = \frac{1}{2}(n + l)$. For $v = 1$, obtain a rectangle (Li, Be), for $v = 2$, a series of rectangles (K, Ca),(Al – Ar); for $v = 3$, a series of rectangles (Cs, Ba),(In – Xe),(Y–Cd), and so on. Table 5.2 shows the diagonal series with odd $n + l$ placed in odd vertical columns and diagonal series with even $n + 1$ in even vertical columns. Now, the odd and, correspondingly, even columns of Table 5.2 form a table of the same structure as in Table 5.1. In both tables, the columns are numbered by v (instead of n) and quantum numbers l, m, s remain the same. Each of them can therefore be related to representation $\{T_{u,C}\}$ in the same sense as it was done with Table 5.1. We therefore get *two* equivalent representations of group SU(2) × SO(4,2). To specify the new arrangement of the elements, define $l = \lambda$, $m = \mu$, $s = \sigma$; for instance, in the "odd" table, *N* is numbered as $(v = 2, \lambda = 1, \mu = 0, \sigma = -1/2)$, Cr as $(v = 3, \lambda = 2, \mu = -1, \sigma = 1/2)$; in the "even" table, Cl is numbered as $(v = 2, \lambda = 1, \mu = 1, \sigma = -1/2)$ and *U* as $(v = 4, \lambda = 3, \mu = -2, \sigma = 1/2)$. In Table 5.2, "odd" and "even" tables are combined, so that the columns of the "odd" table are labeled by numbers $\delta = -\frac{1}{2}$, and the columns of the "even" table are labeled by numbers $\delta = \frac{1}{2}$. In fact, looking at Table 5.1 "along the diagonal" gives exactly Table 5.2.

The rule to fill Table 5.2 is also "lexicographic":

1) The elements are arranged in the order of increasing atomic number *Z*.
2) The sets $(v, \delta, \lambda, \mu, \sigma)$ are arranged in order of increasing v; for fixed v, in order of increasing δ; for fixed v, δ, in order of *decreasing* λ; for fixed v, δ, λ, in order of increasing μ; and for fixed v, δ, λ, μ, in order of increasing σ.
3) *Z*th element corresponds to the *Z*th set.

Table 5.2: A table obtained from Table 5.1 by looking "along the diagonal".

	$\nu = 1$		$\nu = 2$		$\nu = 3$		$\nu = 4$		
	$\delta = -1/2$	$\delta = 1/2$	$\delta = -1/2$	$\delta = 1/2$	$\delta = -1/2$	$\delta = 1/2$	$\delta = -1/2$	$\delta = 1/2$	
$\lambda = 0$	H He	Hi Be	Na Mg	K Ca	Rb Sr	Cs Ba	Fr Ra		$\sigma = -1/2$ $\sigma = 1/2$ } $\mu = 0$
$\lambda = 1$	B C	Al Si	Ga Ge	In Sn	Tl Pb				$\mu = -1$
	N O	P S	As Se	Sb Te	Bi Po				$\mu = 0$
	F Ne	Cl Ar	Br Kr	J Xe	At Rn				$\mu = 1$
$\lambda = 2$			Sc Ti	Y Zr	Lu Hf	Lr Ku			
			V Cr	Nb Mo	Ta W				
			Mn Fe	Tc Ru	Re Os				
			Co Ni	Rh Pd	Ir Pt				
			Cu Zn	Ag Cd	Au Hg				
$\lambda = 3$					La Ce	Ac Th			
					Pr Nd	Pa U			
					Pm Sm	Np Pu			
					Eu Gd	Am Cm			
					Tb Dy	Bk Cf			
					Ho Er	Es Fm			
					Tm Vb	Md No			

Evidently, the elements of Table 5.2 satisfy this rule. If we succeed in interpreting $\nu, \delta, \lambda(\lambda+1), \mu, \sigma$ as quantum numbers of some group, the above numeration will be free of the defect of Madelung numeration implying unnatural combinations like $n + l$. Fixing $\delta = -\frac{1}{2}$ or $\delta = \frac{1}{2}$, we obtain a basis $|\nu, \lambda, \mu, \sigma\rangle$ exactly the same as basis $|n, l, m, s\rangle$ of the space F^2. Thus, we actually have two copies of the space which we denote F^{2-} and F^{2+}; a representation of group SU(2) × SO(4,2) is defined in each of them the same way it was done in Section 3 for a representation in space F^2. However, the obtained representation acts separately in each of the spaces F^{2-}, F^{2+} and does not connect them with each other, so that *two* vectors with $\delta = -1/2$ and $\delta = 1/2$ correspond

to each set of quantum numbers $(\nu, \lambda, \mu, \sigma)$; but number δ has not yet a group-theoretical interpretation. So, another "doubling" of the space is needed. It will be done the same way as in the previous section. Consider vectors

$$X = \begin{bmatrix} \Theta_1 \\ \Theta_2 \end{bmatrix} \tag{5.73}$$

which can be considered as *four-component functions* of $\xi_1, \xi_2, \xi_3, \xi_4$ (as Θ_1, Θ_2 are two-component, see eq. (5.55)). Introduce a scalar product in space F^4 of vectors X. For

$$X = \begin{bmatrix} \Theta_1 \\ \Theta_2 \end{bmatrix}, \quad Y = \begin{bmatrix} T_1 \\ T_2 \end{bmatrix}, \tag{5.74}$$

define

$$\langle X|Y\rangle = \langle \Theta_1|T_1\rangle + \langle \Theta_2|T_2\rangle, \tag{5.75}$$

(where scalar products on the right are taken in spaces F^{2-}, F^{2+}). Proceeding from the representation $\{T_{u,C}\}$ of group SU(2) × SO(4,2) defined in space F^2, we construct now a representation of the group in space F^4

$$G = \mathrm{SU}(2)' \times \mathrm{SU}(2) \times \mathrm{SO}(4, 2) \tag{5.76}$$

where SU(2)′ is another copy of SU(2) group. To do this, it is enough to repeat the procedure (5.65) and (5.66):

$$T_{u',u,C}X = X', \tag{5.77}$$

where

$$\begin{aligned} X &= \begin{bmatrix} \Theta_1 \\ \Theta_2 \end{bmatrix}, \quad X' = \begin{bmatrix} \Theta_1' \\ \Theta_2' \end{bmatrix}, \quad u' = (u'_{\sigma\tau}), \\ \Theta'_\sigma &= \sum_{\tau=1}^{2} u'_{\sigma\tau} T_{u,C}(\Theta_\tau) \end{aligned} \tag{5.78}$$

Operators $T_{u',u,C}$ are related to $T_{u,C}$ the same way as $T_{u,C}$ to T_C and repetition of the above reasoning shows that eqs. (5.77) and (5.78) *define an irreducible unitary representation* of G.

Group G is the group of symmetry of chemical elements. Operator $\sigma'_3 \times 1 \times 1$ of its Lie algebra has eigenvalues $\delta = \pm\frac{1}{2}$ belonging to eigenvectors

$$X_+ = \begin{bmatrix} \Theta \\ 0 \end{bmatrix}, \quad X_- = \begin{bmatrix} 0 \\ \Theta \end{bmatrix} \tag{5.79}$$

Vectors X_- and X_+ constitute a subspace which can be identified with F^{2-}, and F^{2+}, respectively. Thus, δ can be regarded as a quantum number of group G. Since subgroup

$1 \times SU(2) \times SO(4,2)$ can be identified with $SU(2) \times SO(4,2)$, numbers $\nu, \lambda(\lambda+1), \mu, \sigma$ are also quantum numbers of group G. Consequently, the addresses of the element in Table 5.2 are indicated by *sets of quantum numbers of group G* to number basis vectors of space F^4

$$|\nu, \delta, \lambda, \mu, \sigma\rangle. \tag{5.80}$$

As will be shown in the next section, the additional quantum number δ introduced from algebraic considerations is essential for the mass formula for atomic weights, which justifies the second "doubling" of the representation space.

Denoting τ_k, τ'_k the generators of the Lie algebra of groups SU(2) and SU(2)′, respectively, the action of operators to represent them in space F^4 is given by (see eq. (5.71)):

$$\begin{aligned}
&\tau_+\left|\nu, \delta, \lambda, \mu, -\frac{1}{2}\right\rangle = \left|\nu, \delta, \lambda, \mu, \frac{1}{2}\right\rangle, \tau_-\left|\nu, \delta, \lambda, \mu, \frac{1}{2}\right\rangle = \left|\nu, \delta, \lambda, \mu, -\frac{1}{2}\right\rangle,\\
&\tau_3|\nu, \delta, \lambda, \mu, \sigma\rangle = \sigma|\nu, \delta, \lambda, \mu, \sigma\rangle\\
&\tau'_+\left|\nu, -\frac{1}{2}, \lambda, \mu, \sigma\right\rangle = \left|\nu, \frac{1}{2}, \lambda, \mu, \sigma\right\rangle, \tau'_-\left|\nu, \frac{1}{2}, \lambda, \mu, \sigma\right\rangle = \left|\nu, -\frac{1}{2}, \lambda, \mu, \sigma\right\rangle,\\
&\tau'_3|\nu, \delta, \lambda, \mu, \sigma\rangle = \delta|\nu, \delta, \lambda, \mu, \sigma\rangle
\end{aligned} \tag{5.81}$$

whereas operators of Lie algebra of SO(4) act only on quantum numbers ν, λ, μ according to eq. (5.40), n, l, m being replaced by ν, λ, μ.

Now construct the chain of symmetry subgroups (eq. (5.76)). Fixing the unity in group SU(2), obtain subgroup $1 \times SU(2) \times SO(4,2)$. Further, taking subgroup SO(4) of group SO(4,2), as described in Section 5.2, obtain subgroup $1 \times SU(2) \times SO(4)$; the elements of this subgroup are completely defined by matrix u from SU(2) and by four-dimensional rotation $O^{(4)}$ from SO(4). Omitting factor 1, denote this group G_1:

$$G_1 = SU(2) \times SO(4) \tag{5.82}$$

Since each of the spaces F_n is irreducible for SO(4), operators J_k, K_k of its Lie algebra carry each vector (eq. (5.80)) into the vectors generating F_n (see eq. (5.37)). These operators do not change δ, σ. On the other hand, operators $\tau_\pm$, belonging to the complex envelope of the Lie algebra of SU(2), change $\sigma = -1/2$ to $1/2$ and vice versa. Thus, each column of Table 5.2 is the basis of an irreducible representation of G_1, which defines the reduction of the basic representation $\{T_{u',u,C}\}$ of G to G_1.

To obtain the next subgroup of the symmetry chain, take subgroup SO(3) in SO(4,2) as described in Section 5.2; the group

$$G_2 = SU(2) \times SO(3) \tag{5.83}$$

consisting of elements defined by a matrix u from SU(2) and a three-dimensional rotation $O^{(3)}$ from SO(3) is a subgroup of G_1. Operators SO(3) act on μ and do not change all other quantum numbers (see Section 5.3); in particular, $J_\pm + K_\pm$ increase, while corr.

decrease μ by one. On the other hand, operators $\tau_{\pm}$ of SU(2) increase, corr. decrease σ by one. Therefore, each rectangle of Table 5.2 is a basis of an irreducible representation of G_2, and the reduction of basic representation of G to subgroup G_2 is therefore obtained.

Thus, the group chain is

$$G = \mathrm{SU}(2) \times \mathrm{SU}(2) \times \mathrm{SO}(4, 2) \supset \mathrm{SU}(2) \times \mathrm{SO}(4) \supset \mathrm{SU}(2) \times \mathrm{SO}(3) \tag{5.84}$$

(where SU(2)′ is replaced by SU(2) in the first factor of G, that is, for the second copy of SU(2) introduced above). The chain of groups (5.84) defines the *symmetry of the system of elements* and is considered as a key result of our theory. In Chapter 6, the symmetry will be compared with experimental data in detail, and now note some evidence to support the choice of the group chain (5.84). According to the general principles of particle classification discussed in Section 4.7, reduction of the basic representation of the symmetry group G to the consequent subgroups of the chain provides a natural decomposition of the particle multiplet into smaller multiplets connected with each other by some common properties. Later the role of subgroup G_1 will be discussed, and now consider multiplets of subgroup G_2 imaged by vertical rectangles of Table 5.2. Evidently, their elements constitute well-known *s*-, *p*-, *d*-, and *f*-families. In particular, lanthanides and actinides naturally come from our classification as multiplets of subgroup G_2; thus, our group-theoretical approach removes the inappropriate cohabitation of each of these families in the same cell of traditional tables, and each element occupies a unique cell defined by its "address" in the table $(\nu, \delta, \lambda, \mu, \sigma)$, that is, by the corresponding set of quantum numbers of the symmetry group. So, the atoms of all possible elements are put in a one-to-one correspondence with the vectors of the orthonormal basis (eq. (5.80)) in the space of the basic representation of the symmetry group G. According to the classification principles (Section 4.7), these basis vectors represent the states of a system with definite mass; that is, they are eigenvectors of a mass operator. Such operator will be constructed in the next section.

Some more comments are needed about the multiplets of G_2 subgroup. As Table 5.2 shows, not all actinides are present in the multiplet $(\nu = 4, \delta = {}^1\!/_2, \lambda = 3)$: according to the proposed classification, Lr and Ku already start a new family $(\nu = 4, \delta = {}^1\!/_2, \lambda = 2)$. Thus, actinides are divided into families which should be manifested in their properties when new transuranic elements are discovered. Moreover, our classification excludes Lu from the family of lanthanides $(\nu = 4, \delta = {}^{-1}\!/_2, \lambda = 3)$.[47] It belongs to the family $(\nu = 4, \delta = {}^{-1}\!/_2, \lambda = 2)$ along with Hf, Ta, and so on.

47 The conventional model of electron shells leads to the same conclusion, see Landau and Lifshitz (1972, p. 321).

5.5 Mass formula for atomic weights

The mass formula for atomic weights of elements is similar to Gell-Mann–Okubo formula discussed in Section 4.5 for the masses of hadrons which are multiplets of the SU(3) group. For hadrons, each multiplet SU(3) is divided into isotopic multiplets, that is, multiplets of subgroup SU(2), and masses of particles inside these multiplets are very close to each other compared to the differences between isotopic multiplets. Owing to this fact, the mass formula for hadrons consists of two terms (not counting the "unsplit" mass of the multiplet M_0): summand M_1 (see eq. (4.40)) to give average masses of isotopic multiplets, and a smaller summand (see eq. (4.41)) to give the deviation of masses of separate hadrons from average masses of isotopic multiplets which contain them.

Atomic weights of elements are not similar to hadron masses because elements cannot be divided into groups with close masses similar to isotopic multiplets. Assuming that the smallest multiplets of our symmetry, that is, those of subgroup G_2, should play the same role as isotopic multiplets in SU(3) symmetry, it can be assumed that "average" atomic weights of these multiplets (*s*-, *p*-, *d*-, and *f*-families) are to be described by a formula similar to eq. (4.40) for average masses of isotopic multiplets. Large dispersion of masses within each of the families indicates a greater symmetry breaking than in the case of hadrons. More surprising of all is that the average atomic weights of rectangles in Table 5.2 demonstrate an obvious regularity. The very idea of looking for a regularity of average masses is suggested by the analogy with mass formulas for hadrons. Since we do not know how to describe the dispersion of masses within G_2 multiplets, suppose that their "average" masses, characterizing "nonsplit" multiplets G_2, are equal to arithmetic mean values of the masses of elements to form the multiplets. In Table 5.3, these mean values are framed by squares.

Table 5.3: A table with mean values of elements to form the multiplets.

	$v = 1$				$v = 2$				$v = 3$				$v = 4$	
	$\delta = -1/2$		$\delta = 1/2$		$\delta = -1/2$		$\delta = 1/2$		$\delta = -1/2$		$\delta = 1/2$		$\delta = -1/2$	$\delta = 1/2$
$\lambda = 0$	**2,5**	5,5	**8,0**	15,7	**23,7**	15,9	**39,6**	47,0	**86,6**	48,5	**135,1**	89,4	**224,5**	
					8,4		7,4		10,0		11,6		14,3	
$\lambda = 1$					**15,3**	16,9	**32,2**	44,4	**76,6**	46,9	**123,5**	86,7	**210,2**	
									21,3		23,6		22,2	
$\lambda = 2$									**55,3**	44,6	**99,9**	88,1	**188,0**	
													33,4	
$\lambda = 3$													**154,6**	89,8 **244,4**

It can be seen that the differences between these mean masses (the squares in the same horizontal row) are approximately proportional to numbers 1,1,3,3,5,5,… (with the exception of the first one), whereas the vertical differences are proportional

to numbers 1,2,3,… The stabilization is especially noticeable for greater v. A mass formula to describe this regularity can be written as

$$M = m_0 + a \cdot \left[\delta(2v-3) - 5v + \frac{11}{2} + 2(v^2-1)\right] - b \cdot \lambda(\lambda+1) \tag{5.85}$$

where m_0, a, b are theoretically nondeductive factors (similar to those in the mass formula for groups SU(3), SU(6)). Some combinations of quantum numbers in eq. (5.85) are eigenvalues of Casimir operators: $v^2 - 1$ is the value of Casimir operator of group SO(4) (see Section 2.2) and, therefore, of subgroup G_1; and $\lambda(\lambda–1)$is the value of Casimir operator of group SO(3) and, therefore, of subgroup G_2. Varying v, δ, and λ, mass differences obeying the above laws are obtained.

As each of the horizontal differences in Table 5.3 occurs twice, the mass formula should necessary include the evenness of the column of Table 5.4 expressed by the quantum number δ; thus, the replacement of Madelung numeration made above from algebraic considerations introduces exactly those quantum numbers which are required by the experiment.

Table 5.4: Mean masses of multiplets.

λ	$v = 1$		$v = 2$		$v = 3$		$v = 4$
	$\delta = ½$	$\delta = -½$	$\delta = ½$	$\delta = -½$	$\delta = ½$	$\delta = -½$	$\delta = ½$
0	8,16	24,2	40,3	88,5	136,6	216,9	297,2
1		14,3	30,3	78,5	126,7	207,0	287,3
2				58,7	106,9	187,2	267,5
3						157,4	237,7

For $m_0 = 8.0$, $a = 16.1$, $b = 5.0$, we obtain from eq. (5.85) mean masses of multiplets (v, δ, λ) indicated in Table 5.4. As is seen from Tables 5.3 and 5.4, formula (5.85) describes 18 masses by three parameters; except the multiplet (1, $^{-1}/_2$, 0) (containing *H* and *He*), the accuracy of the description is comparable with that obtained for meson octets. This justifies (5.85) as the mass formula for atoms of chemical elements in the same sense as Gell-Mann–Okubo and Beg-Singh (1964) formulas for hadrons. Formula (5.85) is also in a good agreement with the known *P–N* curve to image the dependence between the number of protons and neutrons (Fig. 5.1).

Heavier masses of multiplets are better described by eq. (5.85) which is to be considered as "asymptotic." For $m_0 = 1$, $a = 17$, $b = 5.5$, we obtain from eq. (5.85) the following average atomic weights for "heavy" elements (Table 5.5).

These values can be compared with those of Table 5.3. The numbers in parentheses are predicted average atomic weights of the multiplets of transuranic elements; for example, for multiplet (4, $^1/_2$, 2), starting with Lr and Ku, the average atomic weight should be 274.

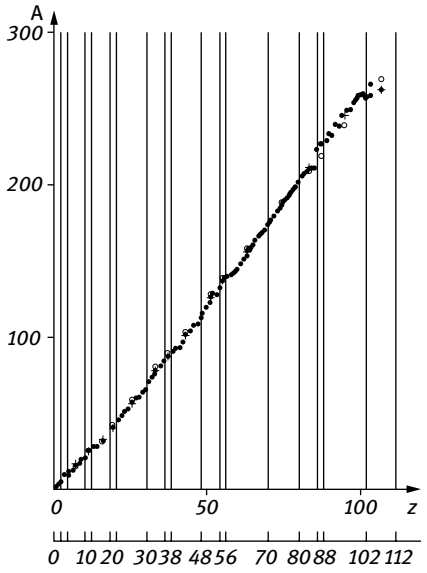


Fig. 5.1: The dependence between the number of protons and neutrons. Average values of m for multiplets are imaged by (+), the values according to mass formula (O), and multiplets ν, δ, λ associated with P equal to the average atomic number of its elements (•). $N = A - P$, where A is the average atomic weight of the elements.

Table 5.5: Average atomic weights for "heavy" elements.

	3,−1/2	**3,1/2**	**4,1/2**	**4,1/2**
0	86	137	222	(307)
1	75	126	211	(296)
2	53	104	189	(274)
3	–	–	156	241

This point of view on the mass formula (5.85) can be compared with Wigner's SU(4) symmetry for heavy nuclei (Wigner, 1932) unacknowledged for a long time. As it turned out these last years, this symmetry is "restored" starting from about $A = 120$. Note that eq. (5.85) also becomes quite accurate for these values A.[48] In addition, the difference between individual atomic weights of heavy elements is also stabilized as is seen from the differences between atomic weights of the elements with $\nu = 3, \lambda = 1$ and $\nu = 3, \lambda = 2$ when δ changes from 1/2 to –1/2. This allows predicting not only

48 The group SU(4) is algebraically kindred to the conformal group: both have isomorphic complex envelops of their Lie algebras.

average values but also individual atomic weights of trans-uranium elements. For the above case, the difference of atomic weights is 88.6. According to eq. (5.85), as the differences corresponding to the change from $\nu = 4, \delta = {}^{-1}/_{2}$ to $\nu = 4, \delta = {}^{1}/_{2}$ should be the same, it is possible to predict atomic weights of ekafrancium Fr′, ekaradium Ra′, and so on, which stand in Table 5.4 on the right of Fr, Ra, … Compare the obtained values with the predictions of Seaborg (1969) based on the shell model:

Table 5.6: Predictions of atomic weights by Seaborg (1969) based on the shell model.

	Fr′	Ra′	Tl′	Rb′	Bi′	Po′	At′	Rn′
Formula 1	312	315	293	296	298	299	299	311
Seaborg	315	316	297	298	–	–	311	314

In the cases considered by Seaborg, a notable difference was found for At′ only. For *Ku* = Hf′, we obtain from eq. (5.85) number 265, whereas Seaborg's prediction was 272; the experimental value is 261. For Ta′ ($Z = 105$), formula (5.85) gives $A = 270$. When compared with experimental data, it should be borne in mind that mass numbers for transuranic elements are found for lighter (neutron-deficit) isotopes, whereas the mass formula relates apparently to the most stable isotopes with higher mass numbers.

6 Classification and chemical properties of elements

6.1 Small multiplets and chemical properties

To describe chemical properties in detail, the above symmetry is to be modified. Namely, we add group G_3 to the group chain $G \supset G_1 \supset G_2$ (eq. (5.84)) to define the symmetry of the system of elements. According to eq. (5.83), $G_2 = \mathrm{SU}(2) \times \mathrm{SO}(3)$. Since groups SU(2) and SO(3) are locally isomorphic (group are considered here from the local viewpoint), there is an isomorphism φ between their vicinities of the unity. To construct it, set a correspondence between generators $J_k + K_k$ of group SO(3) and generators τ_k of group SU(2): then the isomorphism can be defined by

$$\varphi\left(e^{-i[\alpha_1(J_1+K_1)+\alpha_2(J_2+K_2)+\alpha_3(J_3+K_3)]}\right) = e^{-i(\alpha_1\tau_1+\alpha_2\tau_2+\alpha_3\tau_3)} \tag{6.1}$$

(see eq. (3.154)).

Isomorphism φ makes it possible to construct a subgroup of G_2 composed of elements

$$u \times O, \text{ where } u = \varphi(O) \tag{6.2}$$

(see eq. (3.153)). This is exactly the required subgroup G_3. According to the definition of the product of groups,

$$(\varphi(O_1), O_1) \cdot (\varphi(O_2), O_2) = (\varphi(O_1)\varphi(O_2), O_1O_2) = (\varphi(O_1O_2), O_1O_2) \tag{6.3}$$

elements G_3 are multiplied like those of SO(3). Thus, G_3 is locally isomorphic to SO(3), and we denote this subgroup $\mathrm{SO}(3)_C$ (where index C indicates its chemical significance).

Reduction of the basic presentation $\{T_{u',u,C}\}$ of group G to subgroup G_2 provides representation $\{T_{u,O}\}$ to act on vector $\Theta = \begin{bmatrix}\Psi_1\\ \Psi_2\end{bmatrix}$ of space $\mathbb{F}^2$ as follows:

$$T_{u,O}\begin{bmatrix}\Psi_1\\ \Psi_2\end{bmatrix} = \begin{bmatrix}\Psi'_1\\ \Psi'_2\end{bmatrix}, \text{ where } \Psi'_\sigma = \sum_{\tau=1}^{2} u_{\sigma\tau}T_O(\Psi_\tau) \tag{6.4}$$

(see eq. (5.66)). If u is replaced by $\varphi(O)$ and SO(3), SU(2) are considered as two copies of group SO(3), from eq. (3.146), obtain a tensor product of two representations of SO(3): a two-dimensional representation φ and a representation $\{T_O\}$ in the Fock space. As discussed in the end of Section 3.5, this tensor product can be considered as a representation of the subgroup $\mathrm{SO}(3)_C$ obtained by reducing of the basic representation onto this subgroup (see eq. (5.62)):

$$T_{(\varphi(O),O)}(z \otimes \Psi) = (T_{\varphi(O)}z) \otimes T_O\Psi \tag{6.5}$$

This representation acts separately on the components of vector X, i.e. leaves quantum number δ unchanged. Representation (6.5) corresponds to mathematical description of rotations used in atomic physics in the case of "strong spin–orbit coupling" (see eq. (4.7)).

Lie algebra of SO(3) has generators

$$q_k = \tau_k + J_k + K_k \tag{6.6}$$

(see eq. (3.152)) represented in space F^4 by eqs. (5.40) and (5.71).

As mentioned in Section 5.4, representation (6.4) of group $G_2 = \mathrm{SU}(2) \times \mathrm{SO}(3)$ decomposes into irreducible representations numbered by sets of quantum numbers (ν, δ, λ) and imaged by rectangles of Table 5.2. Each of them is defined by a fundamental representation SU(2) (which can be viewed as a two-dimensional irreducible representation of SO(3)) and $(2\lambda + 1)$-dimensional irreducible representation of SO(3). As a result of the reduction to $\mathrm{SO}(3)_C$, we obtain a tensor product of irreducible representations with $j_1 = \frac{1}{2}$ and $j_2 = \lambda$, for which the Clebsch–Gordan sequence $|j_1 - j_2|, \ldots, j_1 + j_2$ consists of two terms $\lambda - \frac{1}{2}, \lambda + \frac{1}{2}$ for $\lambda > 0$ and one term $\frac{1}{2}$ for $\lambda = 0$. Consequently, representation (ν, δ, λ) of group G_2 reduces for $\lambda > 0$ to two irreducible representations of subgroup $G_3 = \mathrm{SO}(3)_C$ with dimensions $2\left(\lambda - \frac{1}{2}\right) + 1 = 2\lambda$ and $2\left(\lambda + \frac{1}{2}\right) + 1 = 2\lambda + 2$, and for $\lambda = 0$ to one two-dimensional irreducible representation (i.e. in this case, the initial two-dimensional representation remains irreducible). Thus, for $\lambda > 0$, multiplets of subgroup G_2 are reduced to two multiplets of subgroup G_3 (Table 6.1). As for all representations of SO(3), quantum numbers $\iota_\lambda = \lambda - \frac{1}{2}$ and $\iota_\lambda = \lambda + \frac{1}{2}$ are introduced for irreducible representations of $\mathrm{SO}(3)_C$ to give the dimensions of these representations $2\lambda = 2\iota_\lambda + 1$ and $2\lambda + 2 = 2\iota_\lambda + 1$, respectively; of course, the "authentic" quantum numbers are values $\iota_\lambda(\iota_\lambda + 1)$ of the Casimir operator of group $\mathrm{SO}(3)_C$

$$\sum_{k=1}^{3} q_k^2 = \sum_{k=1}^{3} (\tau_k + J_k + K_k)^2. \tag{6.7}$$

Thus, the chain of groups

$$G = \mathrm{SU}(2) \times \mathrm{SU}(2) \times \mathrm{SO}(4, 2) \supset \mathrm{SU}(2) \times \mathrm{SO}(4) \supset \mathrm{SU}(2) \times \mathrm{SO}(3) \supset \mathrm{SO}(3)_C, \tag{6.8}$$

has been constructed, which is an extension of the chain (5.84).

According to the principles of particle classification discussed in Section 4.7, the vectors of the selected basis, corresponding to the particles of our system, should belong to the smallest multiplets of the symmetry, that is, the multiplets of subgroup $\mathrm{SO}(3)_C$. This means that vectors $|\nu, \delta, \lambda, \mu, \sigma\rangle$ constructed in Section 5.4 cannot form a selected basis as μ, σ are no longer quantum numbers of the symmetry and the above vectors do not belong to multiplets of G_3. The basis is changed as follows: as ν, δ, λ are associated with groups G, G_1, G_2, they remain quantum numbers of chain (6.8), and new quantum numbers associated with G_3 are introduced instead of μ, σ. One of them, ι_λ, is associated with the Casimir operator of subgroup G_3. The other quantum number, χ, is an eigenvalue of operator $q_3 = \tau_3 + J_3 + K_3$ belonging to the Lie algebra of

$G_3 = \mathrm{SO}(3)_C$. As for multiplets $\mathrm{SO}(3)_C$, number ι_λ is half-integral and χ runs through the following half-integral values:

$$\chi = -\iota_\lambda, -\iota_\lambda + 1, \ldots, \iota_\lambda - 1, \iota_\lambda, \text{ where } \iota_\lambda = \lambda - \frac{1}{2}, \lambda + \frac{1}{2}. \tag{6.9}$$

Quantum numbers ν (associated with the eigenvalues of the Casimir operator of $\mathrm{SO}(4)$), δ (eigenvalue of a generator of $\mathrm{SU}(2)'$), λ (associated with the eigenvalue $\lambda(\lambda+1)$ of the Casimir operator of $\mathrm{SO}(3)$, and ι_λ(associated with eigenvalue $\iota_\lambda(\iota_\lambda+1)$ of the Casimir operator of $\mathrm{SO}(3)_C$) define an irreducible subspace $(\nu, \delta, \lambda, \iota_\lambda)$ of group $\mathrm{SO}(3)_C$ represented by rectangles of Table 6.1. Take normed eigenvectors in this subspace

$$|\nu, \delta, \lambda, \iota_\lambda, \chi\rangle \tag{6.10}$$

of operator q_3, where χ takes values (6.9). By definition, vectors (6.10) belong to "small" multiplets of the group chain (6.8) and form a special basis for this chain.

Thus, extension of the chain group to define the symmetry of the system changes the selected basis whose vectors should represent the elements. The change is like a so-called "mixing" of particles in hadron multiplets (see chains (4.32) and (4.38) in $\mathrm{SU}(3)$ symmetry). In the case of the system of elements, different bases also serve to describe the properties of different elements. However, mass formula (5.85) contains only quantum numbers ν, δ, λ included also in the new set of quantum numbers (eq. (6.10)), so that the description of atomic weights with the agreed accuracy (i.e. average atomic weights of (ν, δ, λ) multiplets) is compatible also with the extended chain (6.8).

The new basis requires new rules of filling the table of elements, that is, a new correspondence

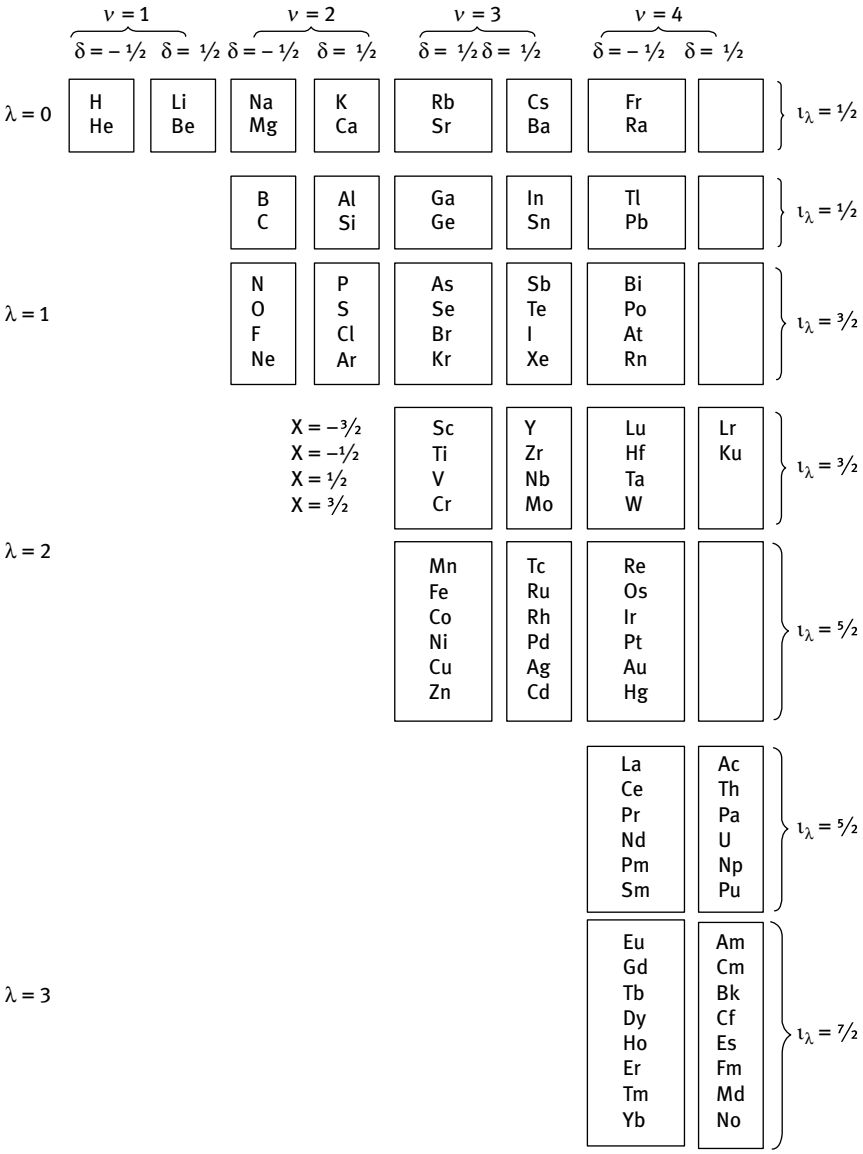
$$Z \leftrightarrow (\nu, \delta, \lambda, \iota_\lambda, \chi). \tag{6.11}$$

"Lexicographic rule" takes now the following form:

(1) The elements are arranged in order of increasing Z;
(2) The sets $(\nu, \delta, \lambda, \iota_\lambda, \chi)$ are arranged in order of increasing ν; for fixed ν, in order of increasing δ; for fixed ν, δ, in order of decreasing λ; for fixed ν, δ, λ, in order of increasing ι_λ; for fixed $\nu, \delta, \lambda, \iota_\lambda$, in order of increasing χ.
(3) Z-th element is put in correspondence to the Z-th set.

The set $(\nu, \delta, \lambda, \iota_\lambda, \chi)$ is the "address" of the element to determine its place in Table 5.4. Evidently, symbols of elements in Table 6.1 satisfy the above rule. Mention again that atomic number Z is not a quantum number in our theory and even is not its part and is considered as an experimental characteristic of an element; the lexicographic rule establishes a correspondence between this characteristic and the sets of quantum numbers to define natural numeration of elements in our symmetry. Thus, quantum numbers are not observables and the rule is introduced as a link with the experiment.

Table 6.1: Periodic table representing multiplets of subgroup G_2 reduced to two multiplets of subgroup G_3.



The multiplets of the subgroups G_1, G_2, G_3 represented by columns, pairs of adjacent rectangles, and separate rectangles of Table 6.1 define the hierarchic classification of chemical elements corresponding to the group symmetry (eq. (6.8)). The naturalness of this classification is primarily due to the fact that multiplets (ν, δ, λ) of subgroup G_2 coincide with known $s-$, $p-$, $d-$ and $f-$ families of elements. Quantum number λ defines the number of elements $4\lambda + 2$, and δ describes the so-called "secondary periodicity" of elements.

To understand the meaning of "small multiplets," that is, multiplets of subgroup G_3, we start from a general idea of how the properties of quantum particles are described in their quantum classification.

If a quantum theory agrees with experimental facts, we can expect that every measurable property P of the particles described by the theory should be expressed by a "regular," that is, analytically correct function of the quantum numbers of the theory. Of course, the group-theoretical approach cannot describe these dependencies quantitatively, but it can indicate some qualitative patterns common to *all* properties. For example, when one of the quantum numbers changes while others remain fixed, property P should naturally depend on the selected quantum number, and the dependence should change abruptly when one of the fixed numbers varies, as quantum numbers change discretely.

In the case of symmetry (eq. (6.8)), the dependencies should have the form

$$P = P(\nu, \delta, \lambda, \iota_\lambda, \chi). \tag{6.12}$$

For different properties P, this dependency may be different and is usually unknown. But we can predict some quantitative characteristics of *all* functions P. For example, assume that values $\nu, \delta, \lambda, \iota_\lambda$ are fixed: $\nu = \nu_1, \delta = \delta_1, \lambda = \lambda_1, \iota_\lambda = \iota_{\lambda 1}$; then by changing χ obtain from eq. (6.12) some regular function $P_1(\chi)$. If now numbers $\nu, \delta, \lambda, \iota_\lambda$ are changed as $\nu = \nu_2, \delta = \delta_2, \lambda = \lambda_2, \iota_\lambda = \iota_{\lambda 2}$, another function $P_2(\chi)$ is obtained. In other words, in respect to the function $P(\chi)$, the remaining quantum numbers play the role of parameters, and discrete change of one of them dramatically changes the form of $P(\chi)$. If $\nu, \delta, \lambda > 0$ are fixed (i.e. in conventional terms, $p-$, $d-$ or $f-$ family of elements), then dependency $P(\chi)$ should change dramatically when ι_λ changes from $\lambda - \frac{1}{2}$ to $\lambda + \frac{1}{2}$. This can manifest itself as a "gap" in the graph, its maximum, and so on, on the border between two small multiplets with the same λ. In Table 6.1, these "transitions" are designated by narrow spaces between adjacent rectangles (with the same λ but different ι_λ).

For the lanthanides family, such division into two subfamilies with different laws of changing properties was first observed by Gaissinsky et al. (1969). We now see that this separation is a common law related to the group symmetry: *each $p-$, $d-$, or $f-$ family of $4\lambda + 2$ elements is divided into subfamilies of 2λ and $2\lambda + 2$ elements in order of increasing atomic numbers, and the dependency of any measurable property of an element on its atomic number changes from the first subfamily to the second*.

To compare this conclusion with experimental data, we considered various properties of elements, including those usually associated with their chemical behavior: ionization potentials; atomic volumes; enthalpy of formation; polarizability of the atoms; boiling point; melting point; heat of evaporation; electron affinity; energy of ionic lattices; dissociation energies of diatomic molecules; and dissociation energies of lanthanide compounds. All experimental data confirm symmetry (6.8). Below there are some typical graphs (Figs. 6.1–6.8) to illustrate the change of regularities between small multiplets; the border to separate them is marked as a dashed line. Apparently, this pattern was not seen before and, in any case, had no explanation.

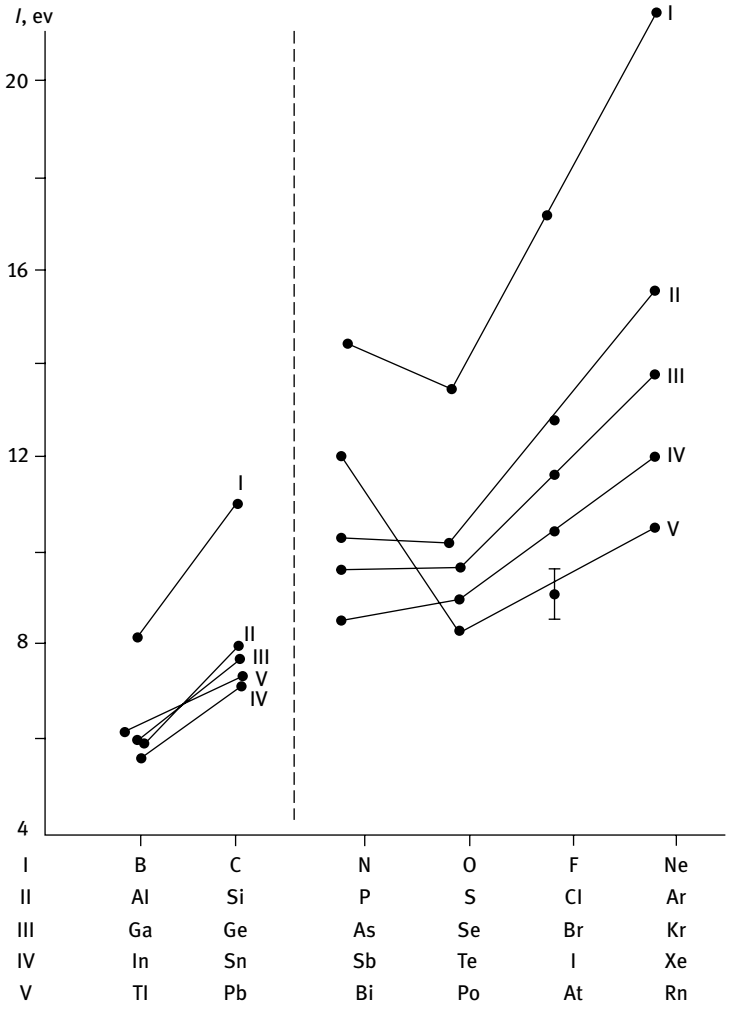


Fig. 6.1: First ionization potentials.

The division of the families into subfamilies described in Rumer and Fet (1971) (see table on p. 208)] was first compared with experimental data by Byakov et al. (1976). The graphs were selected by Sorokin who chose the most important properties of elements.

6.2 Operators of chemical affinity

The larger part of the program to classify particles outlined in Section 4.7 is ready. Now find affinity operators to carry particles with similar properties into each other.

According to Section 4.7, these operators must commute with some subgroup of symmetry group which is a member of the group chain (6.8). Take subgroup $G_2 = SU(2) \times SO(3)$. We will show that operators Γ_+, Γ_- (see eq. (5.52)) commute with this subgroup. In fact, from commutation relations of the conformal group (eq. (5.32)), it follows that

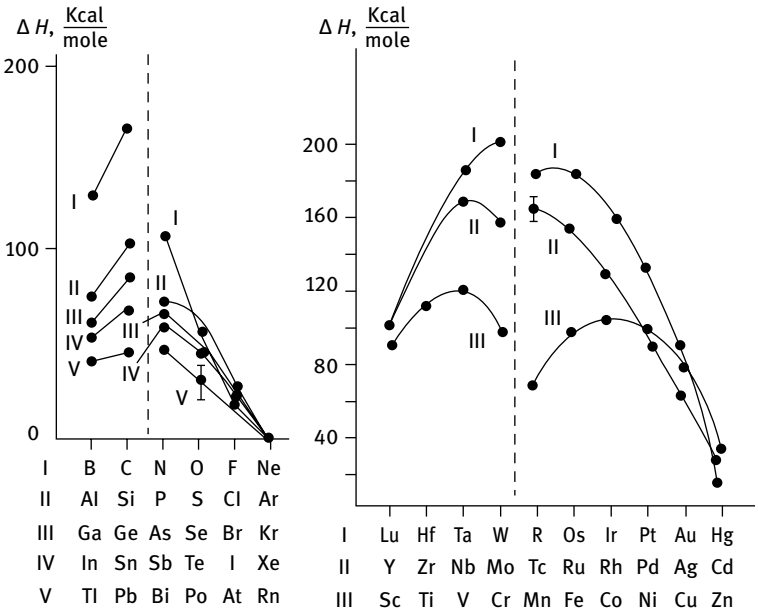


Fig. 6.2: Enthalpies of element formation.

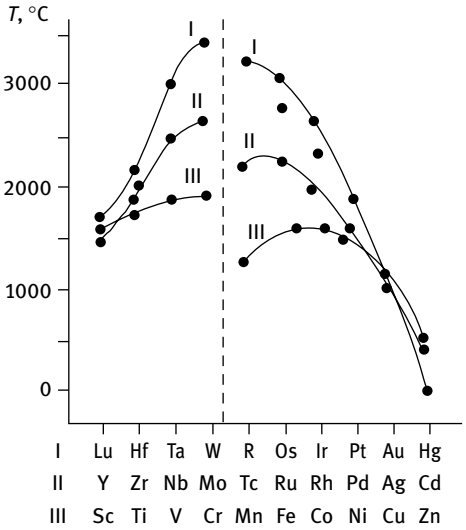


Fig. 6.3: Melting temperatures.

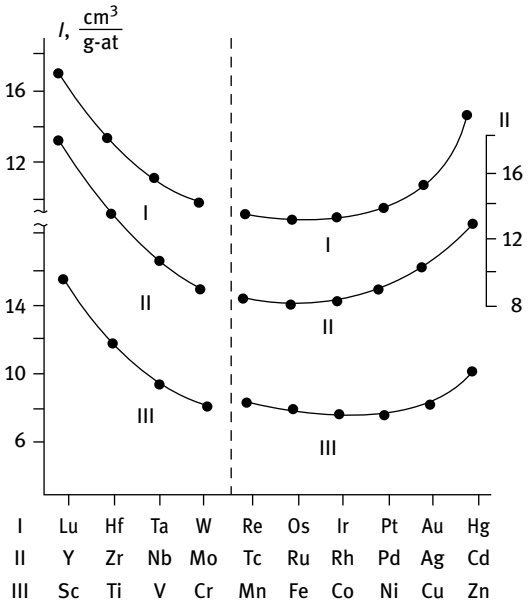


Fig. 6.4: Atomic volumes.

$$[P_{\pm} + Q_{\pm}, J_{+} + K_{+}] = [P_{\pm} + Q_{\pm}, J_{-} + K_{-}] = [P_{\pm} + Q_{\pm}, J_{3} + K_{3}] = 0. \tag{6.13}$$

Hence Γ_{+}, Γ_{-} preserve quantum number μ. Further, Γ_{+}, Γ_{-} commute with the Casimir operator $(J_1 + K_1)^2 + (J_2 + K_2)^2 + (J_3 + K_3)^2$ of subgroup SO(3) and thereby preserve quantum number λ. On the other hand, $\Gamma_{+} = P_{+} + Q_{+}$ and $\Gamma_{-} = P_{-} + Q_{-}$ commute with the operators of subgroup SU(2) and, hence, with $\tau_k (k = 1, 2, 3)$, and therefore, preserve quantum number σ. Since Γ_{+} and Γ_{-} commute with $J_k + K_k$ and τ_k separately, they commute with the subgroup $G_2 = \mathrm{SU}(2) \times \mathrm{SO}(3)$. Further, Γ_{+}, Γ_{-} commute with subgroup SU(2)′, and therefore, preserve quantum number δ. Finally, as was shown in Section 5.3, Γ_{+} carries F_n into F_{n+1}, and Γ_{-} carries F_n into F_{n-1}; therefore, operators Γ_{+}, Γ_{-} in space F^4 increase or, respectively, decrease quantum number ν by 1.

We prove that for all basis vectors,

$$\Gamma_{+}|\nu, \delta, \lambda, \iota_{\lambda}, \chi\rangle \neq 0. \tag{6.14}$$

First, prove a similar statement for the vectors of the previous basis $\upsilon = |\nu, \delta, \lambda, \mu, \sigma\rangle$. Such vector belongs to the irreducible subspace of G_2 defined by values ν, δ, λ. Take $j = \frac{\nu - 1}{2}$ and expand υ in the basis of an irreducible subspace of SO(4) with the same ν, δ (omitting quantum numbers σ, δ):

$$\upsilon = \sum_{\alpha,\beta} \vartheta_{\alpha\beta} |j, \sigma_{\alpha}, \tau_{\beta}\rangle, \tag{6.15}$$

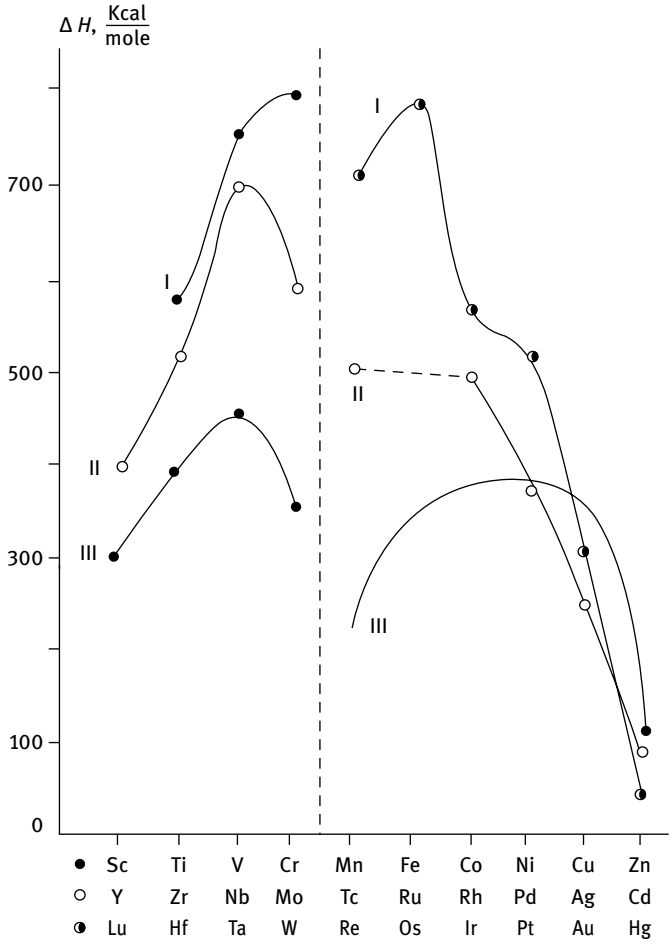


Fig. 6.5: Evaporization heats.

where only the terms with nonzero coefficients $\vartheta_{\alpha\beta}$ are retained. Since υ is an eigenvector of operator $J_3 + K_3$ with eigenvalue μ, we have $\sigma_\alpha + \tau_\beta = \mu$ for all α, β (see eq. (5.37)). Take the term with the largest value σ_α (and, therefore, the smallest value τ_β). Now apply operator Γ_+ to the vector (eq. (6.15)). According to eq. (5.53), we obtain vector $|j + \frac{1}{2}, \sigma_\alpha + \frac{1}{2}, \tau_\beta - \frac{1}{2}\rangle$ with a nonzero coefficient. This vector cannot be reduced by other terms as it has the largest value σ_α. Since basis vectors $|j + \frac{1}{2}, \sigma_\alpha, \tau_\beta\rangle$ are orthogonal, we have $\Gamma_+|\nu, \delta, \lambda, \mu, \sigma\rangle \neq 0$. As shown above, Γ_+ preserves the quantum numbers $\delta, \lambda, \mu, \sigma$ and increases ν by 1; therefore, $\Gamma_+|\nu, \delta, \lambda, \mu, \sigma\rangle = \eta|\nu + 1, \delta, \lambda, \mu, \sigma\rangle$, where $\eta \neq 0$. Apply operators $J_+ + K_+, J_- + K_-, \tau_+, \tau_-$ to the previous equation; it is easily seen from eq. (5.37) (where the coefficients on the right depend only on λ but not on ν, δ) and eq. (5.81) that η does not depend on μ, σ. Thus Γ_+ carries orthonormal basis vectors $|\nu, \delta, \lambda, \mu, \sigma\rangle$ into corresponding basis vectors $|\nu + 1, \delta, \lambda, \mu, \sigma\rangle$ multiplied by η, and is therefore an

isomorphic mapping of the space of multiplet (ν, δ, λ) to the space $(\nu + 1, \delta, \lambda)$ multiplied by $\eta \neq 0$. Since vector $|\nu, \delta, \lambda, \iota_\lambda, \chi\rangle$ belongs to the first of these two spaces, inequality (eq. (6.21)) is proven. So, we have

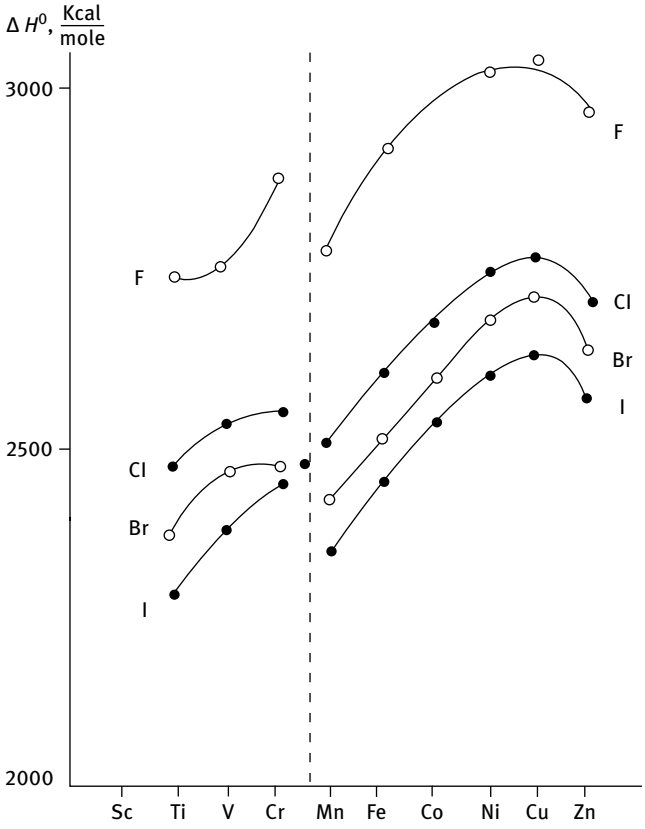


Fig. 6.6: Lattice energy of M^{+2} halogenides.

$$\Gamma_+|\nu, \delta, \lambda, \iota_\lambda, \chi\rangle = \eta|\nu + 1, \delta, \lambda, \iota_\lambda, \chi\rangle, \tag{6.16}$$

where $\eta \neq 0$.

Now show that

$$\Gamma_-|\nu, \delta, \lambda, \iota_\lambda, \chi\rangle \neq 0, \textit{ for } 0 \leq \lambda \leq \nu - 2. \tag{6.17}$$

As P_k and Q_k are Hermitian operators, Γ_+ and Γ_- are Hermitian conjugate operators in space F^4; we have for any vectors υ, w of this space,

$$\langle \Gamma_+ \upsilon | w\rangle = \langle \upsilon | \Gamma_- w\rangle. \tag{6.18}$$

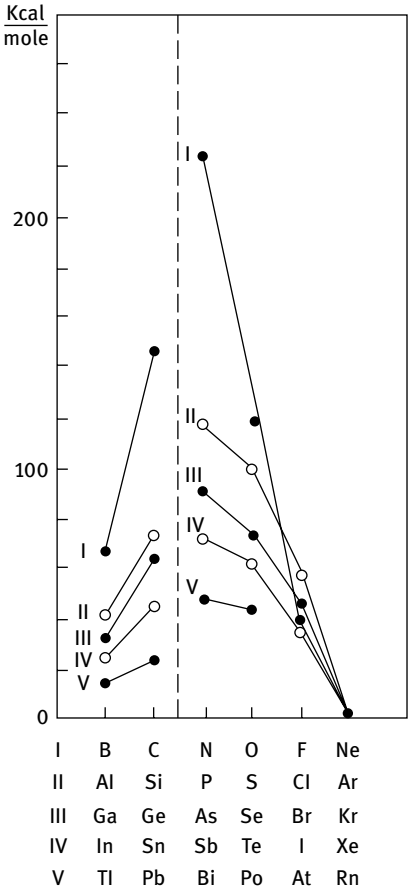


Fig. 6.7: Dissociation energies of diatomic molecules.

Take $\upsilon = |\nu - 1, \delta, \lambda, \iota_\lambda, \chi\rangle$, $w = |\nu - 1, \delta, \lambda, \iota_\lambda, \chi\rangle$, where $0 \le \lambda \le \nu - 2$; since for the values of quantum number $\nu - 1$, the number λ takes values $0, 1, \ldots, (\nu - 1) - 1$, there is a multiplet $(\nu - 1, \delta, \lambda)$, and therefore, vector υ belongs to the basis of space F^4. Similarly, vector w also belongs to this basis. According to eq. (6.16), $\Gamma_+\upsilon = \eta' w$, where $\eta \neq 0$, so that the left side of eq. (6.18) is nonzero and we obtain $\Gamma_- w \neq 0$.

Intuitively operators Γ_+, Γ_- are interpreted as those to transfer basis vectors depicted by the cells of Fig. 6.1 to the right and left, respectively, along the horizontal lines of the table. Specifically, Γ_+ always transfers a basis vector of the column (ν, δ) into a basis vector of a column of the same parity $(\nu + 1, \delta)$, multiplying it by some nonzero factor. Operator Γ_- transfers a basis vector of the column (ν, δ) into a basis vector of a column of the same parity $(\nu - 1, \delta)$, multiplying it by some nonzero factor, provided that the latter exists in the table on the same horizontal (and, as can be shown, into the zero otherwise).

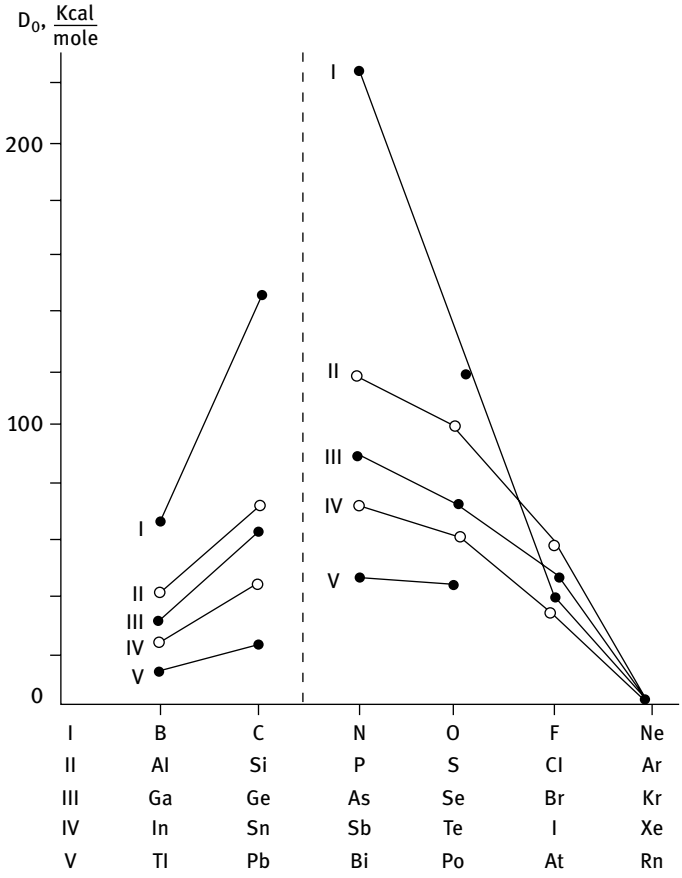


Fig. 6.8: Dissociation energies for lanthanide compounds.

Now show that τ'_+, τ'_- are affinity operators connecting the columns of different parity. Since these operators commute with the subgroup $G_1 = \mathrm{SU}(2) \times \mathrm{SO}(4)$, they preserve quantum numbers $\nu, \lambda, \iota_\lambda, \chi$ related to G_1 and change only quantum number δ (see eq. (5.81)):

$$\begin{aligned} \tau'_+|\nu, {}^{-1}\!/_2, \lambda, \iota_\lambda, \chi\rangle &= |\nu, {}^{1}\!/_2, \lambda, \iota_\lambda, \chi\rangle \\ \tau'_-|\nu, {}^{1}\!/_2, \lambda, \iota_\lambda, \chi\rangle &= |\nu, {}^{-1}\!/_2, \lambda, \iota_\lambda, \chi\rangle \end{aligned} \tag{6.19}$$

The visual interpretation of operators τ'_+, τ'_- is that τ'_+ and τ'_- transfer the basis vectors of each odd and even column, respectively, of Table 6.1 along the horizontal into the basis vectors of the nearest right and left column, respectively. Thus, operators

$$\Gamma_+, \Gamma_-, \tau'_+, \tau'_- \tag{6.20}$$

are affinity operators corresponding to subgroup G_2.

Evidently, horizontal rows of Table 6.1 contain precisely *Mendeleevian homologous series*, that is, family of elements with similar properties. We have singled out these families starting from the general principle of selecting analogs in particle multiplets described in Section 4.7. Therefore, it is natural to call operators (6.20) as *operators of chemical affinity*.

Now the role of subgroup G_1 is clarified: its multiplets contain one representative of each series of Mendeleevian analogs, provided that this series intersects a corresponding column of Table 6.1. *From the viewpoint of the proposed group approach*, *this is the meaning of periodicity*.

As is seen from Table 6.1, homologous series containing the element $|\nu, \delta, \lambda, \iota_\lambda, \chi\rangle$ can intersect only such multiplets of G_1 that $\lambda \leq \nu - 1$. This is what determines the triangular shape of the table. Note that for $\nu = 4, \lambda - 3$, our affinity operators establish a homology between lanthanides and actinides discovered by Seaborg. This homology is thus a special case of the Mendeleevian homology understood in the above sense. On the other hand, we cannot as yet explain the fact that *He* stands in the row of alkaline-earth metals. We hope that quantum numbers of our symmetry will be useful to describe the properties of chemical compounds. Atoms within molecules can be characterized by their quantum numbers. Decomposing the products of corresponding representations of the symmetry group into irreducible representations, we can attempt to classify molecules without analyzing the mechanism of the underlying interaction. Besides this qualitative approach, regularities can be searched in the properties of molecules in terms of quantum numbers of the elements to compose the molecules.

Appendix A. Fock's energy spectrum of the hydrogen atom

A1 Schrödinger equation in the momentum representation

A momentum representation[49] of state vectors is obtained by Fourier transform:

$$\widetilde{\psi}(p) = (2\pi\hbar)^{-3/2}\int \psi(x)e^{-i(px)/\hbar}d^3x, \tag{A.1}$$

where integration is performed over the whole space.

$\widetilde{\psi}(p) = \widetilde{\psi}(p_x, p_y, p_z)$ is a wave function in the momentum representation to represent the same state as $\psi(x)$. The inverse Fourier transform

$$\psi(x) = (2\pi\hbar)^{-3/2}\int \widetilde{\psi}(p)e^{i(px)/\hbar}d^3p \tag{A.2}$$

makes it possible to find $\psi(x)$ from $\widetilde{\psi}(p)$. Plancherel theorem states that Fourier transform preserves scalar products:

$$\langle\widetilde{\psi}|\widetilde{\chi}\rangle = \int \widetilde{\psi}^*(p)\chi(p)d^3p = \int \psi^*(x)\chi(x)d^3x = \langle\psi|\chi\rangle. \tag{A.3}$$

Therefore, mean values and transition probabilities can be calculated in the momentum representation.

Applying momentum operators $p_x = \frac{\hbar}{i}\frac{\partial}{\partial x}, p_y = \frac{\hbar}{i}\frac{\partial}{\partial y}, p_z = \frac{\hbar}{i}\frac{\partial}{\partial z}$ to eq. (A.2), obtain

$$p_x\psi(x) = \frac{\hbar}{i}\frac{\partial}{\partial x}\psi(x) = (2\pi\hbar)^{-3/2}\int p_x\widetilde{\psi}(p)e^{i(px)/\hbar}d^3p, \tag{A.4}$$

and similarly for p_y, p_z. Applying eq. (A.4) once more, obtain operator $p^2 = -\hbar^2\Delta$ in the momentum representation:

$$p^2\psi(x) = (2\pi\hbar)^{-3/2}\int p^2\widetilde{\psi}(p)e^{i(px)/\hbar}d^3p, \tag{A.5}$$

where p^2 under the integral sign is function $p_x^2 + p_y^2 + p_z^2$. This means that Fourier transform of function $p^2\psi(x)$ is $p^2\widetilde{\psi}(p)$; thus, Laplace operator transforms in the momentum representation into the operator of multiplying by p^2.

We will also need the operator of multiplication by $\frac{1}{r}$ in the momentum representation. To do this, find the Fourier integral of $\frac{1}{r}\psi(x)$:

---

49 The term "representation" in this context has nothing to do with group representations and is used here by the tradition of quantum mechanics. Fourier transforms in the forms (A.1) and (A.2) used in quantum mechanics (with factor 1/ħ in exponent) can be converted into the usual form by the change of variables $x = \hbar x'$.

$$\chi(p) = (2\pi\hbar)^{-3/2}\int\frac{1}{r}\psi(x)e^{-i(px)/\hbar}d^3x. \tag{A.6}$$

To facilitate the calculation, introduce factor $e^{-\delta r}(\delta > 0)$ to ensure convergence of intermediate steps:

$$\chi_\delta(p) = (2\pi\hbar)^{-3/2}\int\frac{1}{r}e^{-\delta r}\psi(x)e^{-i(px)/\hbar}d^3x. \tag{A.7}$$

Since $\chi_\delta(p)\to\chi(p)$ for $\delta\to 0$, it is enough to find integral (A.7) for $\delta > 0$. From eq. (A.2), we have

$$\begin{aligned}\chi_\delta(p) &= (2\pi\hbar)^{-3}\int\frac{1}{r}e^{-\delta r}e^{-i(px)/\hbar}d^3x\int\widetilde{\psi}(p')e^{i(p'x)/\hbar}d^3p'\\ &= (2\pi\hbar)^{-3}\int\widetilde{\psi}(p')d^3p'\int\frac{1}{r}e^{-\delta r}e^{i(p'-p)x/\hbar}d^3x.\end{aligned} \tag{A.8}$$

To calculate the inner integral in eq. (A.8), designate $\frac{1}{\hbar}(p'-p) = k$ and introduce spherical coordinates taking direction k as axis z:

$$\begin{aligned}\int\frac{1}{r}e^{-\delta r}e^{ikx/\hbar}d^3x &= \int_0^\infty\int_0^\pi\int_0^{2\pi}\frac{1}{r}e^{-\delta r}e^{ikr\cos\vartheta}r^2\sin\vartheta dr d\vartheta d\varphi\\ &= -2\pi\int_0^\infty re^{-\delta r}dr\int_0^\pi e^{ikr\cos\vartheta}d(\cos\vartheta) = 2\pi\int_0^\infty re^{-\delta r}\frac{e^{ikr}-e^{-ikr}}{ikr}dr\\ &= \frac{4\pi}{k}\int_0^\infty e^{-\delta r}\sin krdr = \frac{4\pi}{k}\frac{k}{k^2+\delta^2} = \frac{4\pi}{k^2+\delta^2},\end{aligned} \tag{A.9}$$

where $k = |p'-p|/\hbar$. Then we have

$$\chi_\delta(p) = \frac{1}{2\pi^2\hbar}\int\widetilde{\psi}(p')\frac{1}{|p'-p|^2+\delta^2\hbar^2}d^3p', \tag{A.10}$$

and for $\delta\to 0$,

$$\chi(p) = \frac{1}{2\pi^2\hbar}\int\frac{\widetilde{\psi}(p')}{|p'-p|^2}d^3p'. \tag{A.11}$$

Apply Fourier transformation to both sides of Schrödinger equation with Coulomb potential[50]:

$$\frac{p^2}{2m}\psi(x) - \frac{Ze^2}{r}\psi(x) = E\psi(x). \tag{A.12}$$

From eq. (A.5) obtain

50 For simplicity, we will say that the electron is considered in the hydrogen atom, though Z is arbitrary here.

$$\frac{p^2}{2m}\widetilde{\psi}(x) - \frac{Ze^2}{2\pi^2\hbar}\int \frac{\widetilde{\psi}(p')}{|p'-p|^2}d^3p' = E\widetilde{\psi}(x). \tag{A.13}$$

Thus, in the momentum representation, Schrödinger equation becomes an *integral equation*.

We need also the following "virial theorem": average values of kinetic and potential energies are related as $2T_{av} = -U_{av}$ for any stationary state of the electron in the Coulomb field. To prove it (see [39, p.234]), mention that that Schrödinger equation (A.12) is equivalent to the variation principle

$$\delta\int \psi^*(T+U-E)\psi d^3x = 0, \tag{A.14}$$

where normalized wavefunctions are varied [35]. Consider, in particular, a special variation $\psi_\lambda(x) = \lambda^{\frac{3}{2}}\psi(\lambda x)$ arising from the similarity transform $x' = \lambda x,\ \ \lambda > 0$. Then ψ_λ are normalized for all λ and by change of variables $x' = \lambda x$, we find

$$\begin{aligned} T_{\lambda av} &= \int \psi_\lambda^*(x) T\psi_\lambda(x) d^3x = \lambda^3 \int \psi^*(\lambda x)\left(-\frac{\hbar^2}{2m}\right)\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)\psi(\lambda x)d^3x \\ &= \lambda^2 \int \psi^*(x')\left(-\frac{\hbar^2}{2m}\right)\left(\frac{\partial^2}{\partial x'^2}+\frac{\partial^2}{\partial y'^2}+\frac{\partial^2}{\partial z'^2}\right)\psi(x')d^3x' = \lambda^2 T_{av}, \end{aligned} \tag{A.15}$$

whence

$$\delta T_{av} = \frac{d}{d\lambda}T_{\lambda av}|_{\lambda=0} = 2T_{av}. \tag{A.16}$$

Assume potential energy $U(x)$ homogeneous of degree ρ, that is, $U(\lambda x) = \lambda^\rho U(x)$. From the calculations similar to eq. (A.15), obtain $U_{\lambda av} = \lambda^{-\rho}U_{av}$ and

$$\delta U_{av} = \frac{d}{d\lambda}U_{\lambda av}|_{\lambda=0} = -\rho U_{av}. \tag{A.17}$$

From eqs. (A.14), (A.16), and (A.17), we have $2T_{av} - \rho U_{av} = 0$ and assuming $\rho = -1$, obtain the theorem to be proved. Therefore, $T_{av} = -E_{av}$ and in the stationary state obtain

$$(p^2)_{av} = -\frac{1}{2m}E. \tag{A.18}$$

Since only bound states are considered, we have $E < 0$.

A2 Fock transformation

Consider four-dimensional *Euclidean* space R^4 with coordinates $\xi_1, \xi_2, \xi_3, \xi_4$ (with no physical meaning). Distance between points $\xi = (\xi_1, \ldots, \xi_4)$ and $\xi' = (\xi'_1, \ldots, \xi'_4)$ in R^4 is given by

$$|\xi - \xi'| = [(\xi_1 - \xi'_1)^2 + \cdots + (\xi_4 - \xi'_4)^2]^{\frac{1}{2}} \tag{A.19}$$

and a unit sphere S^3 centered at the origin is given by

$$\xi_1^2 + \xi_2^2 + \xi_3^2 + \xi_4^2 = 1. \tag{A.20}$$

Introduce spherical coordinates in R^4. Denote ρ the length of the radius vector of the point $\xi = (\xi_1, ..., \xi_4)$ and α its angle with the axis $\xi_4 (0 \le \alpha \le \pi)$. Then $\xi_4 = \rho \cos \alpha$. Designate $r = \rho \sin \alpha$, then r is the length of the projection of this radius vector on plane R^3 ($\xi_4 = 0$), that is, the length of the radius vector of point $\overline{\xi}$ of this plane.

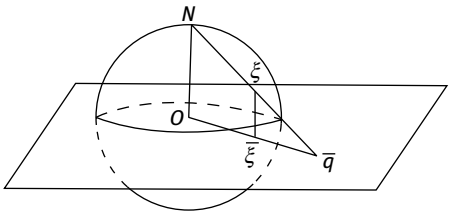


Fig. A.1: Stereographic projection of sphere S^3 on three-dimensional space R^3.

Introduce in R^3 usual spherical coordinates r, ϑ, φ $(0 \le r < \infty, 0 \le \vartheta \le \pi, 0 \le \varphi \le 2\pi)$, then

$$\begin{aligned} \xi_1 &= \rho \sin \alpha \sin \vartheta \cos \varphi \\ \xi_2 &= \rho \sin \alpha \sin \vartheta \sin \varphi \\ \xi_3 &= \rho \sin \alpha \cos \vartheta \\ \xi_4 &= \rho \cos \alpha. \end{aligned} \tag{A.21}$$

Thus, we take ρ $(0 \le \rho < \infty)$, α $(0 \le \alpha \le \pi)$, ϑ $(0 \le \vartheta \le \pi)$, φ $(, 0 \le \varphi \le 2\pi)$ as spherical coordinates in R^4. Also set $\rho = 1$ on the sphere S^3.

Find the area of the unit sphere in R^4. Take on S^3 a surface element $d\Omega$ defined by intervals $(\alpha, \alpha + d\alpha)$, $(\vartheta, \vartheta + d\vartheta)$, $(\varphi, \varphi + d\varphi)$ and project it on plane R^3. The cosine of the angle between the normal to the element area $d\Omega$ and axis ξ_4 is $\xi_4 = \cos \alpha$, so that the projection

$$dS = d\Omega \cos \alpha. \tag{A.22}$$

dS is the three-dimensional volume element in R^3 defined by intervals of spherical coordinates $(r, r + dr)$, $(\vartheta, \vartheta + d\vartheta)$, $(\varphi, \varphi + d\varphi)$, where $r = \sin \alpha$ and, hence, $dr = \cos \alpha d\alpha$. Hereof,

$$dS = r^2 \sin \vartheta dr d\vartheta d\varphi = \sin^2 \alpha \cos \alpha \sin \vartheta d\alpha d\vartheta d\varphi, \tag{A.23}$$

and from eq. (A.22), we have

$$d\Omega = \sin^2\alpha \sin\vartheta d\alpha d\vartheta d\varphi. \tag{A.24}$$

Integrating this expression over the entire sphere S^3, obtain its area

$$\int d\Omega = \int_0^{\pi}\int_0^{\pi}\int_0^{2\pi} \sin^2\alpha \sin\vartheta d\alpha d\vartheta d\varphi = 2\pi^2. \tag{A.25}$$

Fock transformation bases on stereographic projection of sphere S^3 on the three-dimensional space R^3 similar to the projection of a sphere on a complex plane used in the theory of functions (see Fig. A.1). Connect the North Pole of the sphere $(0, 0, 0, 1)$ with its point $\xi = (\xi_1, \xi_2, \xi_3, \xi_4)$ by a plane and intersect this line with plane R^3; the intersection point $\overline{q} = (q_1, q_2, q_3)$ is called a stereographic projection of ξ. From the similarity of triangles $ON\overline{q}$, $\overline{\xi}\xi\overline{q}$ (Fig. A.1) obtain

$$\frac{|\overline{q}|-|\overline{\xi}|}{|\overline{q}|} = \frac{\xi_4}{1} \tag{A.26}$$

(if $\overline{q}$ is inside the sphere, the drawing changes but eq. (A.26) remains true).

Denoting $|\xi_4| = \sqrt{1 - |\overline{\xi}|^2}$, find from eq. (A.26)

$$|\overline{\xi}| = \frac{2|\overline{q}|}{1 + |\overline{q}|^2}, \tag{A.27}$$

since vectors $\overline{\xi}$, $\overline{q}$ have the same direction,

$$\overline{\xi} = \frac{2\overline{q}}{1 + q^2}, \tag{A.28}$$

where $q = |\overline{q}|$. Therefore, taking into account the sign of ξ_4, we have

$$\xi_4 = \frac{q^2 - 1}{q^2 + 1}. \tag{A.29}$$

Thus, we have found the formulas of stereographic projection:

$$\xi_1 = \frac{2q_1}{q^2+1}, \quad \xi_2 = \frac{2q_2}{q^2+1}, \quad \xi_3 = \frac{2q_3}{q^2+1}, \quad \xi_4 = \frac{q^2-1}{q^2+1}. \tag{A.30}$$

Introduce the mean square momentum of the electron in state $\psi(x)$:

$$p_0 = \sqrt{-2mE}, \tag{A.31}$$

where E is the average energy in this state; it is equal to the eigenvalue on the right-hand side of Schrödinger equation (A.12). Use stereographic projection (A.30) to transform sphere S^3 in the momentum space (p_1, p_2, p_3). Define

$$\overline{q} = \frac{\overline{p}}{p_0}, \tag{A.32}$$

then

$$\begin{aligned}
\xi_1 &= \frac{2p_0p_x}{p^2+p_0^2} = \sin\alpha\sin\vartheta\cos\varphi \\
\xi_2 &= \frac{2p_0p_y}{p^2+p_0^2} = \sin\alpha\sin\vartheta\sin\varphi \\
\xi_3 &= \frac{2p_0p_z}{p^2+p_0^2} = \sin\alpha\cos\vartheta \\
\xi_4 &= \frac{p^2-p_0^2}{p^2+p_0^2} = \cos\alpha.
\end{aligned} \tag{A.33}$$

The north pole of S^3 under this transform is carried into the "infinity point" of the momentum space. From eq. (A.30) obtain

$$\sin\alpha = \frac{2q}{q^2+1}, \qquad \sin\alpha d\alpha = -\frac{4qdq}{(q^2+1)^2}, \tag{A.34}$$

and

$$\sin^2\alpha d\alpha = -\frac{8q^2}{(q^2+1)^3}dq \tag{A.35}$$

From eq. (A.24), assuming $d\alpha > 0$, we have

$$d\Omega = \frac{8q^2}{(q^2+1)^3}|dq|\sin\vartheta d\vartheta d\varphi. \tag{A.36}$$

Comparing this expression with the volume element in the momentum space

$$d^3p = p_0^3 d^3q = p_0^3q^2|dq|\sin\vartheta d\vartheta d\varphi, \tag{A.37}$$

we obtain the relation between the elements of three-dimensional volume:

$$d^3p = dp_x dp_y dp_z = \frac{p_0^3}{8}(q^2+1)^3 d\Omega = \frac{(p^2+p_0^2)^3}{8p_0^3}d\Omega. \tag{A.38}$$

Now transform the integral in the Schrödinger equation (A.13) into the integral on the sphere S^3. Express the denominator $|\overline{p}' - \overline{p}|^2$ in terms of the coordinates of points ξ', ξ related to $\overline{p}', \overline{p}$ by eq. (A.33). On one hand,

$$|p' - \bar{p}| = p'^2 + p^2 - 2\bar{p}p' = p_0^2(q'^2 + q^2 - 2\bar{q}q'). \tag{A.39}$$

On the other hand, the square of the distance in four-dimensional space is

$$|\xi' - \xi|^2 = |\bar{\xi}' - \bar{\xi}|^2 + (\xi_4' - \xi_4)^2, \tag{A.40}$$

and from eqs. (A.28) and (A.29), we have

$$
\begin{aligned}
|\xi' - \xi|^2 &= \left| \frac{2\bar{q}'}{1+q'^2} - \frac{2\bar{q}}{q^2+1} \right|^2 + \left(\frac{q'^2-1}{q'^2+1} - \frac{q^2-1}{q^2+1} \right)^2 \\
&= \frac{4}{(1+q'^2)^2(1+q^2)^2}[(q^2+1)\bar{q}' - (1+q'^2)\bar{q}]^2 + \frac{4(q'^2-q^2)^2}{(1+q'^2)^2(1+q^2)^2} \\
&= \frac{4}{(1+q'^2)^2(1+q^2)^2}\{[(1+q^2)^2q'^2+(1+q'^2)^2q^2 - 2(1+q'^2)(1+q^2)\bar{q}\bar{q}'] + (q'^2-q^2)^2\}.
\end{aligned}
\tag{A.41}
$$

After identity transformations, the twisted bracket takes the form

$$
(1+q'^2)(1+q^2)(q'^2+q^2 - 2\bar{q}\bar{q}'), \tag{A.42}
$$

and

$$
|\xi' - \xi|^2 = \frac{4}{(1+q'^2)(1+q^2)}(q'^2+q^2 - 2\bar{q}\bar{q}'). \tag{A.43}
$$

Comparing eq. (A.43) with eq. (A.39), $|\overline{p}' - \overline{p}|$ is expressed in terms of $|\xi' - \xi|$:

$$
|\overline{p}' - \overline{p}| = \frac{p_0^2}{4}(1+q'^2)(1+q^2)\,|\xi' - \xi|^2 = \frac{(p_0^2+p^2)(p_0^2+p'^2)}{4p_0^2}\,|\xi' - \xi|^2. \tag{A.44}
$$

Substituting this into the Schrödinger equation (A.13) and replacing E by $-\frac{p_0^2}{2m}$ (see eq. (A.31)), from eq. (A.38), obtain

$$
\frac{(p^2+p_0^2)}{2m}\widetilde{\psi}(\overline{p}) = \frac{Ze^2}{4\pi^2\hbar p_0}\int \frac{\widetilde{\psi}(\overline{p}')(p_0^2+p'^2)^2}{(p_0^2+p^2)\,|\xi' - \xi|^2}d\Omega'. \tag{A.45}
$$

Multiply eq. (A.45) by $p_0^2 + p^2$ and define a new function on the sphere S^3

$$
\Psi(\xi) = \mu(p^2+p_0^2)^2\widetilde{\psi}(\overline{p}), \tag{A.46}
$$

where $\overline{p}$ should be expressed in terms of ξ from eq. (A.33), and μ is a normalization factor to be chosen, then eq. (A.45) transforms into the following homogeneous integral equation:

$$
\Psi(\xi) = \frac{\lambda}{2\pi^2}\int \frac{\Psi(\xi')}{|\xi' - \xi|^2}d\Omega', \tag{A.47}
$$

where

$$
\lambda = \frac{Ze^2m}{\hbar p_0} = \frac{Ze^2m}{\hbar\sqrt{-2mE}}. \tag{A.48}
$$

The original Schrödinger equation (A.13) is an equation to find the eigenvalues E and corresponding eigenfunctions $\widetilde{\psi}(p)$. Respectively, eq. (A.47) is to find eigenvalues $\frac{\lambda}{2\pi^2}$ and eigenfunctions $\Psi(\xi)$ (factor $1/2\pi^2$ means averaging over the area of sphere S^3, see eq. (A.25)). The two problems are equivalent, since λ is related to E by eq. (A.48), and

$\Psi(\xi)$ is related to $\widetilde{\psi}(p)$ by eq. (A.46). Due to factor $(p^2 + p_0^2)^2$, function $\widetilde{\psi}(p)$ vanishes at $p \to \infty$ provided that $\Psi(\xi)$ remains finite near the north pole of S^3. As will be shown, a very simple form of the transformed eq. (A.47) makes it possible to guess the symmetry group of the Coulomb task.

Now find the normalizing factor μ. From the definition (A.46) of function $\Psi(\xi)$ and from eq. (A.38),

$$\frac{1}{2\pi^2}\int |\Psi(\xi)|^2 d\Omega = \frac{4p_0^3\mu^2}{\pi^2}\int (p^2 + p_0^2)\,|\widetilde{\psi}(\overline{p})|^2 d^3p. \tag{A.49}$$

Since $p_x\widetilde{\psi}(\bar{p})$, $p_y\widetilde{\psi}(\bar{p})$, $p_z\widetilde{\psi}(\bar{p})$ are Fourier transforms of functions $p_x\psi(\bar{x})$, $p_y\psi(\bar{x})$, $p_z\psi(\bar{x})$ (see (A.4)), by theorem (A.3),

$$\begin{aligned}\int p^2|\widetilde{\psi}(p)|^2 d^3p &= \int (p_x^2 + p_y^2 + p_z^2)|\widetilde{\psi}(p)|^2 d^3p \\ &= \int \Big(|p_x\psi(\bar{x})|^2 + |p_y\psi(\bar{x})|^2 + |p_z\psi(\bar{x})|^2\Big) d^3x;\end{aligned} \tag{A.50}$$

due to normalization of $\psi(x)$, the right-hand side of eq. (A.50) is the mean value of $p_x^2 + p_y^2 + p_z^2$, that is, p_0^2. Therefore,

$$\frac{1}{2\pi^2}\int |\Psi(\xi)|^2 d\Omega = \frac{8p_0^5\mu^2}{\pi^2}. \tag{A.51}$$

$$\begin{aligned}\text{If } \mu &= \frac{\pi}{\sqrt{8}} p_0^{-5/2}, \\ \Psi(\xi) &= \frac{\pi}{\sqrt{8}} p_0^{-5/2}(p^2 + p_0^2)^2\widetilde{\psi}(p),\end{aligned} \tag{A.52}$$

the normalization condition for $\Psi(\xi)$ is

$$\frac{1}{2\pi^2}\int |\Psi(\xi)|^2 d\Omega = 1, \tag{A.53}$$

where left-hand side is the average value of $|\Psi|^2$ over S^3. The solutions of integral Fock equation (A.47) are further assumed normalized according to eq. (A.53). In particular, function $\Psi(\xi) \equiv 1$ is normalized in this sense. Since norm preservation results in preserving scalar product, we have

$$\langle\Psi|\Phi\rangle = \frac{1}{2\pi^2}\int \Psi^*(\xi)\Phi(\xi)d\Omega = \int \widetilde{\psi}(\overline{p})^*\widetilde{\varphi}(\overline{p})d^3p = \langle\widetilde{\psi}|\widetilde{\varphi}\rangle = \langle\psi|\varphi\rangle. \tag{A.54}$$

A3 Hydrogen spectrum

We use the classical method of Green's functions to solve the integral (A.47). The solutions will be searched as boundary values of harmonic functions defined in the four-dimensional sphere K^4:

$$\xi_1^2 + \xi_2^2 + \xi_3^2 + \xi_4^2 \le 1. \tag{A.55}$$

A "fundamental solution" of the Laplace's equation $\Delta^4 u = 0$ in the four-dimensional space has singularity in point ξ and can be obtained as follows. Denote $\xi_1, \xi_2, \xi_3, \xi_4$ the coordinates of point ξ and fix them; denote $\xi'_1, \xi'_2, \xi'_3, \xi'_4$ the coordinates of another point $\xi' \neq \xi$ assumed variable. Then function of $\xi'_1, \xi'_2, \xi'_3, \xi'_4$

$$\frac{1}{2|\xi' - \xi|^2} = \frac{1}{2}\frac{1}{(\xi'_1 - \xi_1)^2 + \cdots + (\xi'_4 - \xi_4)^2}, \tag{A.56}$$

where $\xi_1, \xi_2, \xi_3, \xi_4$ are the parameters that satisfy four-dimensional Laplace's equation for $\xi' \neq \xi$.[51] It is readily verified using

$$\frac{\partial}{\partial \xi'_k}|\xi' - \xi| = \frac{\partial}{\partial \xi'_k}\left[\sum_{k=1}^{4}(\xi'_k - \xi_k)^2\right]^{1/2} = \frac{1}{2}\left[\sum_{k=1}^{4}(\xi'_k - \xi_k)^2\right]^{-1/2} \cdot 2(\xi'_k - \xi_k) = \frac{\xi'_k - \xi_k}{|\xi' - \xi|}. \tag{A.57}$$

Now fix point ξ inside K^4 and take another point η by inversion relative to sphere S^3, so that the rays $O\xi, O\eta$ be directed in the same direction and $|\xi||\eta| = 1$. Denote $R = |\xi' - \xi|$, $R_1 = |\xi' - \eta|$, $r = |\xi|$, $r' = |\xi'|$, and designate ω the angle between the rays $O\xi$, $O\xi'$. Function

$$G(\xi, \xi') = \frac{1}{2R^2} + \frac{1}{2R_1^2} \tag{A.58}$$

is called the Green's function of the third order (for the sphere K^4). Being a sum of the two fundamental solutions (with singularities ξ, η), this function of ξ'_k satisfies the four-dimensional Laplace's equation. From the cosine theorem,

$$R^2 = r^2 - 2rr'\cos\omega + r'^2, \quad R_1^2 = \frac{1}{r^2} - \frac{2r'}{r}\cos\omega + r'^2 \tag{A.59}$$

and $G(\xi, \xi')$ for $r' = 1$ (i.e. for point ξ' belonging to S^3) is easily found:

$$G|_{r'=1} = \frac{1}{1 - 2r\cos\omega + r^2}. \tag{A.60}$$

Similarly,

$$\frac{\partial G}{\partial r'}|_{r'=1} = -\frac{1}{1 - 2r\cos\omega + r^2}, \tag{A.61}$$

whence

51 In the space of any dimension $n \ge 3$, the fundamental solution of the Laplace equation has the form $\frac{1}{n-2}\frac{1}{|\xi' - \xi|^{n-2}}$ (where factor $\frac{1}{n-2}$ is used for simplicity). For $n = 3$, this gives the usual fundamental solution $\frac{1}{r}$ known from the elementary potential theory.

$$\left(G + \frac{\partial G}{\partial r'}\right)|_{r'=1} = 0. \tag{A.62}$$

It is the "third-order boundary condition" which gave its name to the Green's function.

Consider now the Green's formula:

$$\int_D (u\Delta v - v\Delta u)dx = \int_\Gamma \left(u\frac{\partial v}{\partial n} - v\frac{\partial u}{\partial n}\right)dS, \tag{A.63}$$

where D is a domain in R^m, dx is a volume element in R^m, Γ is the boundary of D, dS is a surface element of Γ, $\frac{\partial}{\partial n}$ is the differentiation with respect to the outer normal to Γ. This formula is true (and is similarly proved) for any dimension m. Applying it to the domain of K^4_ε obtained from K^4 by excluding from it a ball of small radius ε with center in ξ. Define v as Green's function $G(\xi, \xi')$ (depending on ξ' in a fixed point ξ), and take for u any function of ξ' harmonic in K^4. Respectively, replace in eq. (A.63) dx by $d^4\xi'$, dS by $d\Omega'$, D by K^4_ε. Since both functions u and v are harmonic in K^4_ε, from eq. (A.63) obtain

$$\int_{S^3}\left(u\frac{\partial G}{\partial r'} - G\frac{\partial u}{\partial r'}\right)d\Omega' = -\int_{S^3_\varepsilon}\left(u\frac{\partial G}{\partial n'} - G\frac{\partial u}{\partial n'}\right)d\Omega'_\varepsilon, \tag{A.64}$$

where S^3_ε is the sphere of the radius ε with center in ξ, $d\Omega'_\varepsilon$ is the surface element of the sphere, $\frac{\partial}{\partial n'}$ is the differentiation with respect to the outer normal to K^4_ε, that is, to the inner normal to S_ε. Evidently, $\frac{\partial}{\partial n'} = -\frac{\partial}{\partial R}$ and from eq. (A.59), it follows that for $\varepsilon \to 0$ only the following term is preserved in the right-hand side of eq. (A.64):

$$\lim_{\varepsilon\to 0}\int_{S^3_\varepsilon} u\left(-\frac{\partial}{\partial R}\frac{1}{2R^2}\right)d\Omega_\varepsilon = 2\pi^2 u(\xi) \tag{A.65}$$

(the area of S^3_ε is $2\pi^2\varepsilon^3$). Owing to eq. (A.62), eq. (A.64) takes the form

$$u(\xi) = \frac{1}{2\pi^2}\int_{S^3}\left(\frac{\partial u}{\partial r'} + u\right)|_{r'=1}Gd\Omega'. \tag{A.66}$$

We obtained a representation of harmonic function u in K^4 from boundary values $\frac{\partial u}{\partial r'} + u$. Boundary values G are given by eq. (A.60).

Apply eq. (A.66) to the harmonic polynomial of degree $n-1$, that is, to the homogeneous polynomial of $\xi_1, \xi_2, \xi_3, \xi_4$ of order $n-1$ satisfying the Laplace equation:

$$u = r^{n-1}\Psi_n(\alpha, \vartheta, \varphi) \ \ (n = 1, 2, \ldots), \tag{A.67}$$

where $\Psi_n(\alpha, \vartheta, \varphi)$ is a function on S^3 obtained from the harmonic polynomial for $r = 1$. Then $\frac{\partial u}{\partial r'} = (n-1)r'^{n-2}\Psi_n$ for $n \geq 2$ (0 for $n = 1$),

$$\left(\frac{\partial u}{\partial r'} + u\right)_{r'=1} = n\Psi_n(\alpha', \vartheta', \varphi'), \tag{A.68}$$

and eq. (A.66) takes the form

$$r^{n-1}\Psi_n(\alpha, \vartheta, \varphi) = \frac{n}{2\pi^2}\int_{S^3} \frac{\Psi_n(\alpha', \vartheta', \varphi')}{1 - 2r\cos\omega + r^2} d\Omega'. \tag{A.69}$$

The integral in eq. (A.69) remains valid also for $r = 1$; in this case, the denominator is $|\xi' - \xi|^2$ like in the Fock's integral (A.72). After the limit transition in eq. (A.69) obtain

$$\Psi_n(\xi) = \frac{n}{2\pi^2}\int_{S^3} \frac{\Psi_n(\xi')}{|\xi' - \xi|^2} d\Omega', \tag{A.70}$$

where ξ, ξ' are points of the sphere.

Thus, the boundary values of harmonic polynomials $\Psi_n(\xi)$ or *four-dimensional spherical functions* satisfy the integral Fock's equation with integer eigenvalues $\lambda = n$, $n = 1, 2, \ldots$. It can be proved that these are all solutions of the equation (up to constant factors). In fact, eq. (A.47) is an integral equation with symmetric kernel $\frac{1}{|\xi' - \xi|^2}$, and integral operators with symmetric kernels are Hermitian. Therefore, their eigenfunctions corresponding to different eigenvalues are orthogonal. If there were an eigenfunction (A.47) linearly independent on spherical functions, it could be chosen orthogonal to all spherical functions. But spherical functions can be proved to constitute a complete system S^3, that is, that a function orthogonal to all functions of this system is identically zero. Therefore, Fock's equation is solved. In particular, its eigenvalues are

$$\lambda = n, \quad (n = 1, 2, \ldots).$$

Note that energy eigenvalues E for the hydrogen atoms are related to λ by eq. (A.48) from which the energy spectrum of the hydrogen can be obtained:

$$E_n = -\frac{Z^2 m e^4}{2\hbar^2}\frac{1}{n^2}. \tag{A.71}$$

Thus, the calculation of the energy levels of the electron in the Coulomb field reduces to the solution of the integral Fock's equation (A.47) which surprisingly no longer contains the Coulomb potential. Fock's equation reveals high symmetry of the quantum system associated with this special form of the potential but not directly visible from the Schrödinger equation.

In fact, the representation of the four-dimensional rotation group $\Psi(\xi') = \Psi(O_\xi^{-1})$ (eq. (1.60)) obviously translates a homogeneous harmonic polynomial of degree $n - 1$ $(n = 1, 2, \ldots)$ in polynomials of the same kind and thereby defines a representation of $\mathrm{SO}(4)$ on the space F_n of such polynomials. Later all these representations will be shown irreducible.

Appendix B. Representations of some groups

B1 Local representations of SO(3) and SO(4) groups

Consider some local representation of SO(3) in a finite-dimensional complex vector space C, that is, a representation defined in a vicinity of the identity. We assume that C is a Hilbert space and the representation is unitary.[52] The operators to represent generators A_1, A_2, A_3 of SO(3) group in space C will be denoted by the same letters. Denote $A_+ = A_1 + iA_2,\ A_- = A_1 - iA_2$; then from eq. (3.75), we have the commutation relations

$$[A_3, A_+] = A_+,\ [A_3, A_-] = -A_-,\ [A_+, A_-] = 2A_3. \tag{B.1}$$

The role of operators $A_+,\ A_-$ is seen from the following lemma:

Let eigenvector v of A_3 corresponds to the eigenvalue m. Then A_+v (respectively, A_-v) is an eigenvector A_3 with eigenvalue $m+1$ (respectively, $m-1$) if the vector is not a zero vector. In fact, from eq. (B.1), $A_3(A_+v) = (A_+A_3 + A_+)v = A_+(mv) + A_+v = (m+1)A_+v$ and, similarly, $A_3(A_-v) = (m-1)A_-v$.

Any linear operator in a finite-dimensional space C has eigenvalue (real for Hermitian operators) and finite number of eigenvalues. Designate j the largest eigenvalue of A_3 and v_j the corresponding eigenvector. Then vectors $v_{j-1} = A_-v_j, v_{j-2} = A_-v_{j-1}, \ldots$ (if only they are not zero vectors) are eigenvectors of A_3 with eigenvalues $j-1, j-2, \ldots$. Let this sequence of eigenvectors ends with vector $v_{j'}$ having eigenvalue j'. Then, as we will show,

$$A_+v_m = [j(j+1) - m(j+1)]v_{m+1}, \tag{B.2}$$

where $v_m = 0$ for $m < j',\ m > j$. P prove eq. (B.2) by backward induction with respect to m. For $m = j$, the right-hand side of eq. (B.2) is zero, while the left-hand side becomes zero due to the selection of j and the above lemma. If eq. (B.2) is true for some m, from eq. (B.1), we have

$$\begin{aligned} A_+v_{m-1} = A_+A_-v_m = (A_-A_+ + 2A_3)v_m = A_-([j(j+1) - m(m+1)]v_{m+1}) + 2mv_m \\ = [j(j+1) - m(m+1) + 2m]v_m = [j(j+1) - (m-1)m]v_m, \end{aligned}$$

and eq. (B.2) is therefore true also for $m-1$, which completes the induction.

Now suppose $m = j' - 1$ in eq. (B.2); since j' is the smallest eigenvalue of A_3, obtain $j(j+1) - (j'-1)j' = 0$. For given j, this equation has two solutions, $j' = j+1$ and $j' = -j$. The first of them should be discarded because of the choice of numbers j, j'. So, $j' = -j$, and since $j - j'$ is an integer number, j can have the following values:

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52 It is not a limitation, because in a finite-dimensional space of a representation of a compact Lie group a scalar product can be defined the way that the representation is unitary in the resulting Hilbert space.

$$j = 0, \frac{1}{2}, 1, \frac{3}{2}, 2, \ldots \tag{B.3}$$

So we have vectors $v_{-j}, v_{-j+1}, \ldots, v_{j-1}, v_j$ and

$$\begin{aligned} &A_3 v_m = m v_m, \quad A_- v_m = v_{m-1} (m > -j), \quad A_+ v_m = [j(j+1) - m(m+1)] (m < j), \\ &A_- v_{-j} = 0, \; A_+ v_j = 0. \end{aligned} \tag{B.4}$$

Therefore, $(2j+1)$-dimensional subspace of space C generated by these vectors is irreducible; denote it C_j, and the representation defined by eq. (B.4) denote D_j. If space C is irreducible, then $C = C_j$. Therefore, we have obtained the structure of all local irreducible representations of SO(3).

Normalize vectors v_m by assuming $e_m = v_m / \|v_m\|$. Then from eq. (B.4), we have

$$\langle e_i | A_+ | e_k \rangle = 0 \quad \text{for } i \neq k+1, \; \langle e_i | A_- | e_k \rangle = 0 \quad \text{for } i \neq k-1, \tag{B.5}$$

$$\langle e_i | A_- A_+ | e_k \rangle = 0 \quad \text{for } i \neq k, \; \langle e_m | A_- A_+ | e_m \rangle = j(j+1) - m(m+1). \tag{B.6}$$

Also $A_- = (A_+)^+$, whence $\langle e_m | A_+ | e_{m-1} \rangle = \langle e_{m-1} | A_- | e_m \rangle^*$, and, due to eqs. (B.5) and (B.6), calculation of matrix elements of the product $A_- A_+$ gives

$$\langle e_{m-1} | A_- | e_m \rangle \langle e_m | A_+ | e_m \rangle = |\langle e_{m-1} | A_- | e_m \rangle|^2 = |\langle e_m | A_+ | e_{m-1} \rangle|^2 = j(j+1) - m(m-1).$$

These matrix elements are non-negative. Indeed, vectors e_m differ from v_m only by positive normalizing factors, and from eq. (B.4), we have $A_+ e_m = \lambda e_{m+1}$, $A_- e_m = \mu e_{m-1}$, where $\lambda \geq 0$, $\mu \geq 0$. Therefore, nonzero matrix elements of the A_+, A_- operators are

$$(A_+)_{m,m-1} = (A_-)_{m-1,m} = \sqrt{(j+m)(j-m+1)}. \tag{B.7}$$

Since $A_1 = \frac{1}{2}(A_+ + A_-)$, $A_2 = \frac{1}{2i}(A_+ - A_-)$, find nonzero matrix elements of operators A_k $(k = 1, 2, 3)$:

$$\begin{aligned} (A_1)_{m-1,m} &= (A_1)_{m,m-1} = \frac{1}{2}\sqrt{(j+m)(j-m+1)} \\ (A_2)_{m-1,m} &= -(A_2)_{m,m-1} = \frac{i}{2}\sqrt{(j+m)(j-m+1)} \\ (A_3)_{mm} &= m. \end{aligned} \tag{B.8}$$

Find also the value of Casimir operator $A^2 = A_1^2 + A_2^2 + A_3^2$ of SO(3) group for presentation D_j. Since $A^2 = A_+ A_- + A_3^2 - A_3$ (see eq. (3.131)), from eqs. (B.7) and (B.8), obtain $A^2 e_m = j(j+1) e_m$ for all m, and therefore

$$A^2 v = j(j+1) v \tag{B.9}$$

for all vectors v of space C_j.

Now consider representations of SO(4) group. This group is locally decomposed into a product of subgroups $SO(3)_J$, $SO(3)_K$ (see eq. (5.36)) with generators J_k, K_k ($k = 1, 2, 3$). Find the structure of local irreducible representations of SO(4). Suppose we have a representation of SO(4) in a finite-dimensional Hilbert space C. Generators J_k, K_k are represented in space C by operators which will be denoted by the same letters. Since operators J_3, K_3 are Hermitian and commute with each other (see eq. (5.32)), there is their common eigenvector $e_{m_1^0 m_2^0}$ in C corresponding to the eigenvalues of these operators m_1^0 and m_2^0. Applying operators J_+, J_- of subgroup $SO(3)_J$ to vector $e_{m_1^0 m_2^0}$, obtain, like above, a sequence of eigenvectors e_{-j_1, m_2^0}, e_{-j_1+1, m_2^0}, ..., e_{j_1-1, m_2^0}, e_{j_1, m_2^0} of operator J_3 to constitute a basis of an irreducible subspace C_{j_1} of this subgroup. Since K_3 and J_+, J_- commute, each vector $e_{m_1 m_2^0}$ is also an eigenvector of J_3 with eigenvalue m_1 and eigenvector K_3 with eigenvalue m_2^0. Applying operators K_+, K_- of subgroup $SO(3)_K$ to vector $e_{m_1 m_2^0}$, obtain vectors $e_{m_1 m_2}$ which are simultaneously eigenvectors of J_3, K_3 with corresponding eigenvalues m_1, m_2, unless these vectors are zero vectors.

Now show that the range of change for m_2 for which $e_{m_1 m_2} \neq 0$ does not depend on m_1. In fact, assume $e_{m_1 m_2} \neq 0$, $m_1' \neq m_1$. Then there is such degree p of operator J_+ (or J_-) that $e_{m_1 m_2^0} = \lambda J_\pm^p e_{m_1' m_2^0}$, and such degree q of operator K_+ (or K_-) that $e_{m_1 m_2} = \mu\lambda K_\pm^q J_\pm^p e_{m_1' m_2^0}$, where μ, λ are some nonzero numbers, and sign ± means that both cases are considered simultaneously. From commutation relations, we have

$$e_{m_1 m_2} = \mu\lambda J_\pm^p (K_\pm^q e_{m_1' m_2^0}) = \mu\lambda J_\pm^p e_{m_1' m_2'}, \tag{B.10}$$

and, consequently, $e_{m_1' m_2'} \neq 0$. Applying operator K_3 to both sides of eq. (B.10) and again using commutation relations, obtain $m_2' = m_2$. Therefore, from $e_{m_1 m_2} \neq 0$, it follows that $e_{m_1' m_2'} \neq 0$, which was to be proved.

Assume $m_2 = -j_2, -j_2 + 1, \ldots, j_2 - 1, j_2$. Then vectors $e_{m_1 m_2}$ belong to eigenvalues m_1, m_2 of operators J_3, K_3, respectively. Evidently, operators $J_\pm$, $K_\pm$ convert, up to a numerical factor, these vectors into each other or into the zero. This defines an irreducible subspace of group SO(4) with dimension $(2j_1 + 1)(2j_2 + 1)$. Denote $C_{j_1 j_2}$ this subspace and $D_{j_1 j_2}$ the corresponding representation. If the initial representation of SO(4) group in space C is irreducible, then $C = C_{j_1 j_2}$. On the other hand, representations $D_{j_1 j_2}$ can be constructed for *any* integer or half-integer j_1, j_2:

$$j_1 = 0, \frac{1}{2}, 1, \frac{3}{2}, 2, \ldots; \quad j_2 = 0, \frac{1}{2}, 1, \frac{3}{2}, 2, \ldots \tag{B.11}$$

To do this, it is enough to take a space with basis $e_{m_1 m_2}$, where $m_1 = -j_1, -j_1 + 1, \ldots, j_1 - 1, j_1$ and $m_2 = -j_2, -j_2 + 1, \ldots, j_2 - 1, j_2$, and define operators J_k, K_k by eq. (B.8) so that J_k act on index m_1 and K_k act on index m_2. Thus, we found the structure of all irreducible representations of SO(4) group.

Denoting m_1 as σ, m_2 as τ, and basis vectors $e_{m_1 m_2}$ as $|\sigma, \tau\rangle$, we can see that space $C_{j_1 j_2}$ of representation $D_{j_1 j_2}$ is a tensor product of spaces C_{J_1}, C_{J_2}, where irreducible representations D_{J_1}, D_{J_2} of SO(3) group are defined. The action of operators $J_\pm$, J_3 of subgroup

$SO(3)_J$ on index σ and operators $K_\pm$, K_3 of subgroup $SO(3)_K$ on index τ is defined by eqs. (B.7) and (B.8) to result in eq. (5.37).

Above we discussed Casimir operator $\Lambda^2 = 2(J_1^2 + J_2^2 + J_3^2) + +2(K_1^2 + K_2^2 + K_3^2) = \sum_{\alpha<\beta} Z_{\alpha\beta}^2$ of $SO(4)$ group (see eq. (2.38) where $\hbar$ should be replaced by 1). It can be easily shown that the value Λ^2 for representation $D_{j_1 j_2}$ is $2j_1(j_1+1) + j_2(j_2+1)$; for $j_1 = j_2 = \frac{n-1}{2}$, we obtain $n^2 - 1$.

Another Casimir operator of $SO(4)$ group has the form $M^2 = 2(J_1^2 + J_2^2 + J_3^2) - 2(K_1^2 + K_2^2 + K_3^2)$ and is $2j_1(j_1+1) - 2j_2(j_2+1)$ for presentation $D_{j_1 j_2}$. Thus, both Casimir operators define numbers j_1, j_2 and, therefore, an irreducible representation of $SO(4)$.

B2 Spherical functions and reduction of representations

The Laplace equation is the source of spherical functions. *Harmonic polynomial* of n-th order is a homogeneous polynomial $u_n(x_1, \ldots, x_m)$ of n-th order of m variables and satisfying the Laplace equation:

$$\Delta u_n = \frac{\partial^2 u_n}{\partial x_1^2} + \cdots + \frac{\partial^2 u_n}{\partial x_m^2} = 0. \tag{B.12}$$

Denote r the radius vector of point x in space R^m, $r = (x_1^2 + \cdots + x_m^2)^{1/2}$, then u_n can be written as

$$u_n(x) = r^n Y_n(\xi), \tag{B.13}$$

where $Y_n(\xi)$ is a function on the sphere $S^{m-1}(x_1^2 + \cdots + x_m^2 = 1)$ uniquely defined by polynomial u_n and, in turn, defining this polynomial. Thus obtained function $Y_n(\xi)$ is called an *m-dimensional spherical function of order n*.[53] We will further consider three-dimensional and four-dimensional spherical functions, but some of the simplest results are proved similarly for any dimension m.

We begin with the following theorem the underlying the expansion of functions defined on the sphere by spherical functions:

Let $f_n(x_1, \ldots, x_m)$ be a homogeneous polynomial of degree n. Then there exists a unique harmonic polynomial of the same degree u_n such that

$$f_n = u_n + r^2 f_{n-2}, \tag{B.14}$$

where f_{n-2} is a homogeneous polynomial of degree $n-2$.

Polynomial u_n is called a harmonic projection of polynomial f_n. The proof of the theorem has two parts: first the existence of decomposition (eq. (B.14)) will be proved

53 Note that this term is applied only to functions of a special form which are spherical values of harmonic polynomials rather than to any function defined on sphere S^{m-1}.

and the formula will be derived to find harmonic projection of the given polynomial f_n, and then the uniqueness of the decomposition will be proved.

We will further use a formula for a homogeneous polynomial of order k $f_k(x_1, \ldots, x_m)$:

$$\Delta(r^2 f_k) = 2(m + 2k)f_k + r^2 \Delta f_k \tag{B.15}$$

To prove it, apply the Leibniz rule for differentiating a product to $r^2 f_k$:

$$\Delta(r^2 f_k) = 2mf_k + 4\sum_{j=1}^{m} x_j \frac{\partial f_k}{\partial x_j} + r^2 \Delta f_k. \tag{B.16}$$

According to Euler's theorem on homogeneous functions, $4\sum_{j=1}^{m} x_j \frac{\partial f_k}{\partial x_j} = kf_k$ which results in eq. (B.15). Reapplying eq. (B.15) easily proves the following equation by induction with respect to p:

$$\Delta(r^{2p} f_k) = 2p(m + 2k + 2p - 2)r^{2p-2} f_k + r^{2p} \Delta f_k \quad (p = 1, 2, \ldots) \tag{B.17}$$

and for $k = n - 2p$, obtain

$$\Delta(r^{2p} f_{n-2p}) = 2p(m + 2n - 2p - 2)r^{2p-2} f_{n-2p} + r^{2p} \Delta f_{n-2p} \quad (p = 1, 2, \ldots, 2p \le n) \tag{B.18}$$

Find the harmonic polynomial projection of $f_n(x)$ in the form

$$u_n = \sum_{p=0}^{[n/2]} \alpha_p r^{2p} \Delta^p f_n, \tag{B.19}$$

where Δ^p is the pth degree of the Laplace operator ($\Delta^0 = 1$ is the identity operator), $[n/2]$ is the integer part of number $n/2$, and α_p are undetermined coefficients. The summation in eq. (B.19) is done until $\Delta^p f_n$ becomes zero, that is, $2p \le n$. Apply Laplace operator to both sides of eq. (B.19). Assuming in eq. (B.18) $f_{n-2p} = \Delta^p f_n$, obtain the identity

$$\Delta(r^{2p} \Delta^p f_n) = 2p(m + 2n - 2p - 2)r^{2p-2} \Delta^p f_n + r^{2p} \Delta^{p+1} f_n, \tag{B.20}$$

and

$$\Delta u_n = \sum_{p=0}^{[n/2]} [\alpha_p + (2p + 2)(m + 2n - 2p - 4)\alpha_{p+1}] r^{2p} \Delta^{p+1} f_n, \tag{B.21}$$

where $\alpha_{[n/2]+1} = 0$. The last term vanishes for any f_n as $2(p + 1) > n$ is true in it, the rest terms vanish at any f_n if the recurrence relations are fulfilled:

$$\alpha_p + (2p + 2)(m + 2n - 2p - 4)\alpha_{p+1} = 0 \left(p = 0, \ldots, \left[\frac{n}{2}\right] - 1 \right). \tag{B.22}$$

We assume $n > 0$ since f_0 is a constant with evident expansion (eq. (B.14)) $f_0 = f_0 + r^2 \cdot 0$. Then brackets in eq. (B.22) are positive for all considered values of p, and from eq. (B.22), we consistently find all α_p if α_0 is given. Assume $\alpha_0 = 1$ and find all other α_p according to the above reasoning; then eq. (B.19) defines a *harmonic* polynomial u_n,

the first term in eq. (B.19) is f_n, and the rest of them contain factor r^2 which gives expansion (eq. (B.14)).

Now prove the *uniqueness* of eq. (B.14). First show that the spherical functions of different orders are orthogonal to each other:

$$\int_{S^{m-1}} Y_l^* \xi Y_{l'}(\xi) d\Omega = 0 \, (l \neq l'). \tag{B.23}$$

By definition, $u_l(x) = r^l Y_l(\xi)$ and $u_{l'}(x) = r^{l'} Y_{l'}(\xi)$ are harmonic polynomials of orders l and l', respectively. Apply to them Green's formula in the unit sphere $K^m(x_1^2 + \ldots + x_m^2 \leq 0)$:

$$\int_{K^m} (\Delta u_l^* u_{l'} - u_l^* \Delta u_{l'}) d^m x = \int_{S^{m-1}} \left(\frac{\partial u_l^*}{\partial n} u_{l'} - u_l^* \frac{\partial u_{l'}}{\partial n} \right) d\Omega. \tag{B.24}$$

The left-hand side is zero, and in the right-hand side, differentiation along the outward normal coincides with the differentiation along r: $\frac{\partial u_l}{\partial n} = l r^{l-1} Y_l$, and similarly, $\frac{\partial u_{l'}}{\partial n} = l' r^{l'-1} Y_{l'}$. Introducing it into eq. (B.24) and assuming $r = 1$, we have $(l - l') \int Y_l^* Y_{l'} d\Omega = 0$, whence obtain eq. (B.23) for $l \neq l'$.

The set $H_{m,n}$ of all m-dimensional spherical functions of n-th order is a linear space; since spherical function $Y_n(\xi)$ and harmonic polynomial $u_n(x)$ mutually define each other, this space is isomorphic to the space of polynomials u_n. This space is finite, because it is a subspace of the space of all homogeneous polynomials f_n of order n having a finite basis of monomials $x_1^{r_1} \ldots x_m^{r_m}$. Thus, $H_{m,n}$ is a finite-dimensional space. Choose for each n an orthonormal basis $Y_n^{(1)}, \ldots, Y_n^{(q_n)}$ of space $H_{m,n}$. Then from eq. (B.23), we have

$$\int_{S^{m-1}} Y_l^{(i)*} Y_{l'}^{(j)} d\Omega = \delta_{ll'} \delta_{jj'}. \tag{B.25}$$

Using eq. (B.14), apply the same formula to f_{n-2}: $f_n = u_n + r^2 u_{n-2} + r^4 f_{n-4}$, then to f_{n-4}, and so on, and thus obtain the *canonical decomposition* of the homogeneous polynomial:

$$f_n = u_n + r^2 u_{n-2} + r^4 u_{n-4} + \cdots, \tag{B.26}$$

where $u_n, u_{n-2}, u_{n-4}, \ldots$ are the harmonic polynomials of the respective degrees, and where the right-hand side ends either with the term $r^{2p} u_1$ or the term $r^{2p} u_0$. Assume $r = 1$; designating (f) spherical values of function f, we have

$$(f) = Y_n + Y_{n-2} + \cdots \tag{B.27}$$

We have thus proved that the values of homogeneous polynomial f_n on S^{m-1} can be represented as a sum of spherical functions of order n or lower. Expressing these spherical functions by selected basic functions, obtain the expansion

$$(f_n) = \sum_{n',j} c_{n'}^{(j)} Y_{n'}^{(j)} \, (n' \leq n, j = 1, \ldots, q_{n'}). \tag{B.28}$$

Applying a similar expansion to u_n and f_{n-2} obtain from eq. (B.15):

$$(f_n) = \sum_j c_n^{(j)} Y_n^{(j)} + \sum_{\substack{n' < n \\ j}} c_{n'}^{(j)} Y_{n'}^{(j)}, \tag{B.29}$$

where the first term on the right-hand side, containing spherical functions of order n is (u_n). Multiplying both sides of eq. (B.29) by $Y_n^{(k)*}$ and integrating over S^{m-1}, find from eq. (B.25)

$$c_n^{(k)} = \int_{S^{m-1}} Y_n^{(k)^*}(f_n) d\Omega. \tag{B.30}$$

Thus, all coefficients are uniquely determined by polynomial f_n which defines (u_n) and, finally, u_n. This completes the proof of the decomposition theorem (eq. (B.15)).

We call u_n a harmonic projection of polynomial f_n; assuming $u_n = Pf_n$, easily obtain that P is a *linear* operator: indeed, if $u_n^{(1)} = Pf_n^{(1)}$, $u_n^{(2)} = Pf_n^{(2)}$, then $f_n^{(1)} + f_n^{(2)} = u_n^{(1)} + u_n^{(2)} + r^2(f_{n-2}^{(1)} + f_{n-2}^{(2)})$, and from the uniqueness of eq. (B.15), we have $u_n^{(1)} + u_n^{(2)} = P(f_n^{(1)} + f_n^{(2)})$. Similarly, prove that $P(\lambda f_n) = \lambda P(f_n)$.

Now we can prove that spherical functions constitute a *complete set* of functions on the sphere S^{m-1}. As is known, the completeness of an orthonormal system admits two equivalent formulations: (*a*) any (square-integrable) function can be expanded in a norm convergent series in terms of the functions of the system; (*b*) any (square-integrable) function orthogonal to all functions of the system is zero. We will prove that completeness of the system of spherical functions in the second formulation. Let (f) be a function on S^{m-1} orthogonal to all $Y_l^{(j)}$. As is seen from eq. (B.27), the values of any homogeneous polynomial (f_n) on S^{m-1} are decomposed into a sum of spherical functions. Therefore, (f) orthogonal to all polynomials of $x_1, \ldots, x_m$ (homogeneous or not). Extend (f) to function $f(x_1, \ldots, x_m)$ defined throughout the space R^m and then approximate it by polynomial $f_n(x_1, \ldots, x_m)$ using the Weierstrass theorem. Since function (f) is orthogonal on S^{m-1} to function (f_n) arbitrarily close to (f), then (f) is orthogonal to itself and thereby vanishes. This proves the completeness of the system of spherical functions and the possibility to expand the functions on the sphere in terms of spherical functions. This decomposition is unique because the coefficients can be derived from the orthogonality relations (eq. (B.25)), as it was done above.

Consider now representations of the rotation group $\mathrm{SO}(m)$. For each m, there is a representation of this group in the space of harmonic polynomials $H_{m,n}$:

$$Y'_n = T_o Y_n, \text{ where } Y'(\xi) = Y_n(O^{-1}\xi). \tag{B.31}$$

Denote this representation $T^{(m,n)}$. It can be shown that for $m \geq 3$, all representations $T^{(m,n)}$ are irreducible.[54]

54 A general proof and detailed discussion of representations $T^{(m,n)}$ and multidimensional spherical functions see in B (Vilenkin, 1965, ch. ix). We prove the irreducibility only for $m = 3, 4$ using special properties of these dimensions. For $m = 2$, the representation will be proved reducible.

SO(m) group contains subgroup SO($m-1$) composed of rotations to preserve coordinate x_m. Make a reduction of $T^{(m,n)}$ to this subgroup. Expand the harmonic polynomial $u_n(x_1, \ldots, x_m)$ in powers of x_m; denoting x point $(x_1, \ldots, x_m)$ and x' point $(x_1, \ldots, x_{m-1})$, obtain $u_n(x) = x_m^n f_0(x') + x_m^{n-1} f_1(x') + f_n(x')$. Expand $f_n(x')$ by eq. (B.15): $f_n(x') = v_n(x') + r'^2 f_{n-2}(x')$, where $v_n(x')$ is the harmonic polynomial of $x_1, \ldots, x_{m-1}$ and $r'^2 = x_1^2 + \cdots + x_{m-1}^2$. Replacing r'^2 by $r^2 - (x_m)^2$, represent $u_n(x)$ as $x_m^n f_0^{(1)}(x') + x_m^{n-1} f_1^{(1)}(x') + \cdots + x_m f_{n-1}^{(1)}(x') + v_n(x') + r^2 f_{n-2}(x')$, where $f_j(x')$ is replaced by polynomials of the same order $f_j^{(1)}(x')$. Applying the same method to $f_{n-1}^{(1)}(x')$, and so on, express $u_n(x)$ as

$$u_n(x) = x_m^n v_0(x') + x_m^{n-1} v_1(x') + \cdots + v_n(x') + r^2 f_{n-2}(x'), \tag{B.32}$$

where $v_j(x')$ are harmonic polynomials of $x_1, \ldots, x_{m-1}$.

Expansion (B.32) underlies the reduction. The terms in eq. (B.32) are not, generally speaking, harmonic polynomials of $x_1, \ldots, x_m$, but the required expansion $H_{m,n}$ into irreducible subgroups of subspace SO($m-1$) can be obtained by applying the operator of harmonic projection P to both sides of eq. (B.32). Since $Pu_n = u_n$, $P(r^2 f_{n-2}) = 0$, we have

$$u_n(x) = P(x_m^n v_0(x')) + P(x_m^{n-1} v_1(x')) + \cdots + P(v_n(x')). \tag{B.33}$$

Using eq. (B.19), we can find the form of terms. In fact,

$$\Delta^p (x_m^{n-j} v_j(x')) = \left(\Delta' + \frac{\partial^2}{\partial x_m^2}\right)^p (x_m^{n-j} v_j(x')), \tag{B.34}$$

where Δ' is a (m–1)-dimensional Laplace operator, and since $\Delta' v_j(x') = 0$, the right-hand side of eq. (B.34) is $\alpha_{mnj} x_m^{n-j-2p} v_j(x')$, where α_{mnj} is a numerical factor. From eq. (B.19), we have

$$P(x_m^{n-j} v_j(x')) = \Big(\sum b_{mnjp} r^{2p} x_m^{n-j-2p}\Big) v_j(x'), \tag{B.35}$$

where b_{mnjp} are numerical factors depending only on m, n, j, p, but not on $u_n(x)$. Substitute expression of eq. (B.35) into eq. (B.33), denote $x_m = r\cos\alpha$,where α is the angle between the radius-vector of point x and axis x_m, and, finally, assume $r = 1$. Since $r' = r\sin\alpha$, from eq. (B.33), obtain the expansion of an arbitrary m-dimensional spherical function $Y_n(\xi)$ into the sum of m-dimensional spherical functions of a special form:

$$Y_n(\xi) = \sum_{j=0}^{n} C_{mnj}(\cos\alpha) \cos\alpha \sin^j \alpha Y_j(\xi'), \tag{B.36}$$

where ξ is a point of sphere S^{m-1}, ξ' is a point of sphere $S^{m-2}(x_1^2 + \cdots + x_{m-1}^2 = 1)$, $Y_j(\xi')$ are (m-1)-dimensional spherical functions of order j ($j = 0, 1, \ldots, n$), and $C_{mnj}(z)$ are polynomials of one variable $z = \cos\alpha$ referred to as Gegenbauer polynomials. It can be shown that for $m = 3$, these polynomials coincide (with proper normalization) with known Legendre polynomials, and for $m = 4$, they have the form

$$\text{Const} \cdot \frac{d^{j+1}(\cos(n+1)\alpha)}{d(\cos\alpha)^{j+1}}. \tag{B.37}$$

For all kinds of $(m-1)$-dimensional spherical functions $Y_j(\xi')$ of order j, the j-th term in eq. (B.36) runs through the subspace *invariant with respect to the subgroup* $\mathrm{SO}(m-1)$; in fact, this subgroup acts on ξ' only and converts spherical functions $Y_j(\xi')$ into each other. The vectors of this subspace are completely defined by functions $Y_j(\xi')$, so that it is isomorphic to $H_{m-1,j}$. Thus, the reduction of eq. (B.37) can be written as:

$$H_{m,n} = \bigoplus_{j=0}^{n} H_{m-1,j}. \tag{B.38}$$

Note that we have proved the only invariance of the subspaces in the right-hand side relative to $\mathrm{SO}(m-1)$, while in fact, they are irreducible with respect to this subgroup (for $m \geq 3$).

Consider now in more detail the spherical functions of 1, 2,and 3 variables, that is, spherical values of harmonic polynomials of 2, 3, and 4 variables. Harmonic polynomials of two variables are easy to describe. All homogeneous polynomials of order n of x, y are linear combinations of monomials $x^{n-j}y^j$ ($j = 0, ..., n$). According to eq. (B.14), $P(f_2) = P(g_2)$ is equivalent to the statement that $f_2 - g_2$ divides by $r^2 = x^2 + y^2$. Hence it is easy to deduce that $P(x^{n-j}y^j) = P(x^n)$ for even $j > 0$ and $P(x^{n-j}y^j) = P(x^{n-1}y)$ for odd j, while $P(x^n)$ and $P(x^{n-1}y)$ are not multiples of each other. Consequently, harmonic polynomials of n-th degree ($n > 0$) constitute a two-dimensional space. Assuming $\varsigma = x + iy$, take for basis polynomials $\mathrm{Re}(\varsigma^n)$ (multiple of $P(x^n)$) and $\mathrm{Im}(\varsigma^n)$ (multiple of $P(x^{n-1}y)$) or their linear combinations $\mathrm{Re}(\varsigma^n) + i\mathrm{Im}(\varsigma^n) = \varsigma^n$, $\mathrm{Re}(\varsigma^n) - \mathrm{Im}(\varsigma^n) = (\varsigma^*)^n$.

The action of group $\mathrm{SO}(2)$ on these basis vectors is obvious: denoting T_α the rotation of the plane about angle α, we have

$$T_\alpha(\varsigma^n) = e^{in\alpha}\varsigma^n,\ T_\alpha((\varsigma^*)^n) = e^{-in\alpha}(\varsigma^*)^n, \tag{B.39}$$

For $r = 1$, functions $\varsigma^n = r^n e^{in\varphi}$, $(\varsigma^*)^n = r^n e^{-in\varphi}$ transform into two-dimensional spherical functions $e^{in\varphi}$ ($n = \ldots -2, -1, 0, 1, 2, \ldots$), and the expansion of an arbitrary function defined on sphere S^1 in terms of these functions reduces to expansion of a periodic function into Fourier series. Spherical functions of order n have the basis of two functions

$$Y_n^+(\varphi) = e^{in\varphi},\ \ Y_n^-(\varphi) = e^{-in\varphi}. \tag{B.40}$$

As follows from eq. (B.39), space $H_{2,n}$ decomposes into a sum of two one-dimensional irreducible subspaces generated by functions (B.40) ($n > 0$).

Consider now three-dimensional spherical functions. Using traditional designations, replace in eq.(B.37) α by ϑ, n by l, and j by m; also denote $C_{3lm}(\cos\vartheta)\sin^m\vartheta = c_{lm}P_l^{(m)}(\cos\vartheta)$, where c_{lm} is a normalization factor. Substituting the expressions of two-dimensional spherical functions (B.40) into eq. (B.36), obtain the following decomposition for three-dimensional spherical functions

$$Y_l(\vartheta, \varphi) = c_{l_0} P_l^{(0)}(\cos\vartheta) + \sum_{m=1}^{l} [c_{lm}^{+} P_l^{(m)}(\cos\vartheta) e^{im\varphi} + c_{lm}^{-} P_l^{(-m)}(\cos\vartheta) e^{-im\varphi}], \tag{B.41}$$

where c_{l_0}, c_{lm}^{+}, c_{lm}^{-} are constant factors and $P_l^{(m)}$ are Legendre functions. Since both functions $P_l^{(m)}$, $P_l^{(-m)}$ correspond to the same polynomial C_{3lm}, they can differ only by a numerical factor.

Thus, the basis of space $H_{3,l}$ consists of $2l+1$ functions

$$\begin{aligned} &Y_l^m(\vartheta, \varphi) = P_l^{(m)}(\cos\vartheta) e^{im\varphi} \\ &(l = 0, 1, 2, \ldots; m = -l, -l+1, \ldots, l-1, l). \end{aligned} \tag{B.42}$$

Now show that this space is *irreducible* for the representation $T^{(3,l)}$ of SO(3) group. For $m = l$, obtain the eigenvector of operator $L_{12} = \frac{1}{i}\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) = \frac{1}{i}\frac{\partial}{\partial y}$ corresponding to the eigenvalue l. According to the local theory of representations of group SO(3) (Section 1), the irreducible subspace of space $H_{3,l}$ containing vector $Y_l^{(l)}$ has the dimension no less than $2l+1$. From eq. (B.41), it follows that the number is the dimension of the whole space $H_{3,l}$ which proves the irreducibility of the latter. Thus, odd-dimensional representations of SO(3) group are *globally* realized on the spaces $H_{3,l}$ of spherical functions. These representations of $T^{(3,l)}$ correspond to D_l.

A vice versa, even-dimensional local representation of SO(3) corresponding to *half-integer* values l do not exist as global representations, that is, they cannot be unambiguously continued from a neighborhood of the unity to the whole group SO(3). So-called "double-valued" representations are used in physics instead of these non-existent unique representations. In these representations (which are not representations of a group in the sense defined in Chapter 1), each element of SO(3) (i.e. each rotation O) is associated with *two* operators $\pm T_o$ acting in an even-dimensional space, and either $T_{o_1 o_2} = T_{o_1} T_{o_2}$ or $T_{o_1 o_2} = -T_{o_1} T_{o_2}$ for any choice of signs. In the vicinity of the unity operators, T_o can be chosen uniquely if taken close to the identity operator, then they depend continuously on rotation O. Thus, we again obtain local representations. In the important case of a two-dimensional representation to transform wave-functions with the spin (Section 4.1), the double-valued nature of the representation results in the fact that for "large" rotations, the transformed wave-function is defined only up to the sign, that is, to the phase factor unimportant in quantum mechanics.

Finally, consider four-dimensional spherical functions. Again using expansion (B.36), obtain for the functions of n-th order the following basis (see eq. (1.54)):

$$Y_{nlm}(\alpha, \vartheta, \varphi) = \Pi_{n+1,l}(\alpha) Y_l^{(m)}(\vartheta, \varphi), \tag{B.43}$$

where $l = 0, 1, \ldots, n$ and $m = -l, -l+1, \ldots, l-1, l$ for the given l. It is easy to calculate the number $(n+1)^2$ of basis vectors (eq. (B.43)) and, therefore, the dimension of space $H_{4,n}$. To prove the irreducibility of the space, note that harmonic polynomial $(x_1 + ix_2)^n$ is also the eigenvector of commuting operators $J_3 = \frac{1}{2}(L_{12} - L_{34})$ and $K_3 = \frac{1}{2}(L_{12} + L_{34})$ (see eq. (5.30)) with the same eigenvalue $\frac{n}{2}$. Construct a local representation $D_{j_1 j_2}$ of

SO(4) group from the initial vector $(x_1 + ix_2)^n$ as described in Section 1. Then we have $j_1 \geq \frac{n}{2}$, $j_2 \geq \frac{n}{2}$, so that the dimension $(2j_1 + 1)(2j_2 + 1)$ of irreducible subspace $C_{j_1 j_2}$ is not less than $(n + 1)^2$. Therefore, the dimension is the dimension of the whole space $H_{4,n}$, which thus coincides with $C_{j_1 j_2}$ to prove its irreducibility.

For $m = 4$, obtain from eq. (B.37) the decomposition of the four-dimensional space of spherical functions of order n into irreducible subspaces of subgroup SO(3):

$$H_{4,n} = H_{3,0} \oplus H_{3,1} \oplus \ldots \oplus H_{3,n}. \tag{B.44}$$

The basis function (B.42) is an eigenfunction of operators Λ^2, L^2, and L_3, with eigenvalues $(n + 1)^2 - 1$, $l(l + 1)$ and m, respectively.

B3 Some representations of SU(3) group

Here we construct eight- and ten-dimensional irreducible representations of SU(3) group necessary to understand Section 4.4. The general construction of any representations of SU(3) (and SU(n)) is seen in [24].

The octet representation. First consider a nine-dimensional complex space C^9 with the orthonormal basis:

$$\Psi_\mu^\lambda \ (\lambda, \mu = 1, 2, 3). \tag{B.45}$$

Construct in C^9 a representation of SU(3) group by defining for Okubo matrices A_τ^σ corresponding operators in space C^9 denoted by the same letters:

$$A_\tau^\sigma \Psi_\mu^\lambda = \delta_\mu^\sigma \Psi_\tau^\lambda - \delta_\tau^\lambda \Psi_\mu^\sigma. \tag{B.46}$$

It is easily verified, operators (B.46) satisfy the same commutation relations as Okubo matrices (see eq. (4.30)). Besides, corresponding operators λ_j (see eq. (4.28)) are Hermitian, which is readily verified by writing out their matrix elements; therefore, the constructed representation is unitary.

To find an irreducible subspace of SU(3) group in C^9, note that multiple vectors

$$\Psi_0 = \Psi_1^1 + \Psi_2^2 + \Psi_3^3 \tag{B.47}$$

are carried into zero by all operators A_τ^σ and thereby constitute an invariant subspace C^1 of SU(3) group. Since the operators of the unitary representation carry orthogonal vectors into orthogonal vectors, the orthogonal complement to C^1 in C^8 is also invariant. Denote it

$$C^9 = C^1 \oplus C^8. \tag{B.48}$$

The basis of C^8 consists of the following eight vectors which form an orthonormal system and are therefore linearly independent:

$$\begin{aligned} &e_1 = \Psi^1_3, \quad e_2 = -\Psi^2_3, \quad e_3 = \Psi^1_2, \quad e_4 = \tfrac{1}{\sqrt{2}}(\Psi^1_1 - \Psi^2_2), \\ &e_5 = -\Psi^2_1, \quad e_6 = \tfrac{1}{\sqrt{6}}(2\Psi^3_3 - \Psi^1_1 - \Psi^2_2), \quad e_7 = \Psi^3_2, \quad e_8 = \Psi^3_1 \end{aligned} \tag{B.49}$$

Construct operators T_k of the Lie algebra of subgroup SU(2) (see eq.(4.33)). Denote $T_\pm = T_1 \pm iT_2$; then $T_+ = A^2_1$, $T_- = A^1_2$, $T_3 = A^1_1 + \frac{1}{2}A^3_3$ and from eqs. (B.46) and (B.49),

$$\begin{aligned} &T_+e_1 = e_2, \quad T_+e_2 = 0, \quad T_-e_2 = e_1, \quad T_-e_1 = 0, \quad T_3e_1 = -\frac{1}{2}e_1, \quad T_3e_2 = \frac{1}{2}e_2; \\ &T_+e_3 = \sqrt{2}\,e_4, \quad T_+e_4 = \sqrt{2}\,e_5, \quad T_+e_5 = 0, \\ &T_-e_5 = \sqrt{2}\,e_4, \quad T_-e_4 = \sqrt{2}\,e_3, \quad T_-e_3 = 0, \\ &T_3e_3 = -e_3, \quad T_3e_4 = 0, \quad T_3e_5 = e_5; \\ &T_+e_6 = T_-e_6 = T_3e_6 = 0; \\ &T_+e_7 = e_8, \quad T_+e_8 = 0, \quad T_-e_8 = e_7, \quad T_-e_7 = 0, \quad T_3e_7 = -\frac{1}{2}e_7, \quad T_3e_8 = \frac{1}{2}e_8. \end{aligned} \tag{B.50}$$

As follows from eq. (B.49), space C^8 decomposes into the orthogonal sum of irreducible subspaces of subgroup SU(2) generated, respectively, by vectors e_1, e_2, then vectors e_3, e_4, e_5, then vector e_6 and, finally, vectors e_7, e_8. Denoting these subspaces in the same order C^2, C^3, C^1, $C^{2'}$, we have

$$C^8 = C^2 \oplus C^3 \oplus C^1 \oplus C^{2'}. \tag{B.51}$$

Now prove that the whole space C^8 is irreducible for SU(3) group. To do this, it is sufficient to verify that operators of the Lie algebra of this group interconnect subspaces C^2, C^3, C^1, $C^{2'}$. As is seen from eq. (B.49),

$$\begin{aligned} &A^3_2e_1 = e_3, \quad A^2_3e_3 = e_1; \quad A^3_2e_5 = e_8, \quad A^3_3e_8 = e_5; \\ &A^3_2e_2 - A^3_1e_1 = \sqrt{6}\,e_6; \quad A^1_3e_6 = -\tfrac{\sqrt{6}}{2}e_6, \end{aligned} \tag{B.52}$$

which proves the irreducibility of C^8.

Applying operators A^1_1, A^3_3 to basis vectors, find the following eigenvalues:

	e_1	e_2	e_3	e_4	e_5	e_6	e_7	e_8
A^1_1	−1	0	−1	0	1	0	0	1
A^3_3	1	1	0	0	0	0	−1	−1

(B.53)

The decuplet representation. First consider the complex space C^{27} with the orthonormal basis

$$\Psi_{\lambda\mu\nu} \ (\lambda, \mu, \nu = 1, 2, 3). \tag{B.54}$$

Define a representation of SU(3)group in space C^{27} by

$$\begin{aligned} &A^\sigma_\tau\Psi_{\lambda\mu\nu} = \delta^\sigma_\lambda\Psi_{\tau\mu\nu} + \delta^\sigma_\mu\Psi_{\lambda\tau\nu} + \delta^\sigma_\nu\Psi_{\lambda\mu\tau} \quad (\sigma \neq \tau), \\ &A^\sigma_\sigma\Psi_{\lambda\mu\nu} = \delta^\sigma_\lambda\Psi_{\sigma\mu\nu} + \delta^\sigma_\mu\Psi_{\lambda\sigma\nu} + \delta^\sigma_\nu\Psi_{\lambda\mu\sigma} - \Psi_{\lambda\mu\nu}. \end{aligned} \tag{B.55}$$

Commutation relations (eq. (4.30)) are readily verified, though the calculation is somewhat cumbersome. Operators λ_j are again Hermitian, so the representation is unitary.

The invariant subspace we are interested in is generated by 10 orthonormal vectors built from vectors $\Psi_{\lambda\mu\nu}$ by symmetrization over all indices:

$$\begin{aligned}
&e_1 = \Psi_{333}, \quad e_2 = \tfrac{1}{\sqrt{3}}(\Psi_{233} + \Psi_{323} + \Psi_{332}), \quad e_3 = \tfrac{1}{\sqrt{3}}(\Psi_{133} + \Psi_{313} + \Psi_{331}),\\
&e_4 = \tfrac{1}{\sqrt{3}}(\Psi_{223} + \Psi_{232} + \Psi_{322}), \quad e_5 = \tfrac{1}{\sqrt{6}}(\Psi_{123} + \Psi_{132} + \Psi_{213} + \Psi_{231} + \Psi_{312} + \Psi_{321}),\\
&e_6 = \tfrac{1}{\sqrt{3}}(\Psi_{113} + \Psi_{131} + \Psi_{311}), \quad e_7 = \Psi_{222}, \quad e_8 = \tfrac{1}{\sqrt{3}}(\Psi_{122} + \Psi_{212} + \Psi_{221}),\\
&e_9 = \tfrac{1}{\sqrt{3}}(\Psi_{112} + \Psi_{121} + \Psi_{211}), \quad e_{10} = \Psi_{111}.
\end{aligned} \tag{B.56}$$

Applying operators (eq. (B.54)) to such symmetrical linear combinations gives linear combinations of the same vectors $e_1, \ldots, e_{10}$, so the generated space is invariant (which will be shown below by direct calculation). Denote this space C^{10}.

The operators of the Lie algebra of SU(2) subgroup act on the basis vectors by the formulas following from eqs. (B.55) and (B.56):

$$\begin{aligned}
&T_+e_1 = T_-e_1 = T_3e_1 = 0;\\
&T_+e_2 = e_3, \quad T_+e_3 = 0, \quad T_-e_3 = e_2, \quad T_-e_2 = 0, \quad T_3e_2 = -\tfrac{1}{2}e_2, \quad T_3e_3 = \tfrac{1}{2}e_3;\\
&T_+e_4 = \sqrt{2}\,e_5, \quad T_+e_5 = \sqrt{2}\,e_6, \quad T_+e_6 = 0,\\
&T_-e_6 = \sqrt{2}\,e_5, \quad T_-e_5 = \sqrt{2}\,e_4, \quad T_-e_4 = 0,\\
&T_3e_4 = -e_4, \quad T_3e_5 = 0, \quad T_3e_6 = e_6;\\
&T_+e_7 = \sqrt{3}\,e_8, \quad T_+e_8 = 2e_9, \quad T_+e_9 = \sqrt{3}\,e_{10}, \quad T_+e_{10} = 0,\\
&T_-e_{10} = \sqrt{3}\,e_9, \quad T_-e_9 = 2e_8, \quad T_-e_8 = \sqrt{3}\,e_7, \quad T_-e_7 = 0,\\
&T_3e_7 = -\tfrac{3}{2}e_7, \quad T_3e_8 = -\tfrac{1}{2}e_8, \quad T_3e_9 = \tfrac{1}{2}e_9, \quad T_3e_{10} = \tfrac{3}{2}e_{10}.
\end{aligned} \tag{B.57}$$

This shows that C^{10} decomposes into an orthogonal sum of irreducible subspaces of subgroup SU(2) generated by vector e_1, then by vectors e_2, e_3, then by vectors e_4, e_5, e_6, and, finally, by vectors e_7, e_8, e_9, e_{10}:

$$C^{10} = C^1 \oplus C^2 \oplus C^3 \oplus C^4. \tag{B.58}$$

Since these subspaces are connected by operators (eq. (B.55)) ($\sigma, \tau = 1, 2, 3$), C^{10} is an irreducible space of SU(3) group:

$$\begin{aligned}
&A_2^3e_1 = \sqrt{3}\,e_2, \; A_3^2e_2 = \sqrt{3}\,e_1; \; A_2^3e_2 = 2e_4, \; A_3^2e_4 = \sqrt{3}\,e_2;\\
&A_2^3e_4 = \sqrt{3}\,e_7, \; A_3^2e_7 = \sqrt{3}\,e_4.
\end{aligned} \tag{B.59}$$

The eigenvalues of operators A_1^1, A_3^3 for basis vectors are also found from eq. (B.55):

	e_1	e_2	e_3	e_4	e_5	e_6	e_7	e_8	e_9	e_{10}
A_1^1	−1	−1	0	−1	0	1	−1	0	1	2
A_3^3	2	1	1	0	0	0	−1	−1	−1	−1

(B.60)

References

M. Barrondo, O.A. Novaro, *J. Phys. B* 5 (1972), 1104

A.O. Barut, "Structure of Matter", *Rutherford Centennial Symposium*, New Zealand, 1972.

M. Beg, V. Singh, *Phys. Rev. Lett.* 13 (1964), 113.

V.M. Byakov, Y.I. Kulakov, Y.B. Rumer, A.I. Fet, "*Group-Theoretical Classification of Chemical Elements*", *Preprint of the Institute for Theoretical and Experimental Physics*, parts 1,2, 1976; part 3, 1977.

M.G. Calif, *Inst. of Technology Synchrotron Laboratory Report CTSL-20*, 1961.

P.A.M. Dirac, *Ann. Math.* 36 (1937).

A.I. Fet, *JETP Letters* 20 (1974), 24 [in Russian].

A.I. Fet, *Teoreticheskaya i Matematicheskaya Fizika* 22 (1975), 323 [in Russian].

A.I. Fet, "*The System of Elements from the Group-Theoretic Viewpoint*", *Preprint of the Institute of Inorganic Chemistry SB AS USSR*, 1979a.

A.I. Fet, "The Madelung numbers and the system of chemical elements", *Group theoretical methods in physics, v.I, Proceedings of the International Workshop, Zvenigorod, 1979b, Nauka, Moscow*, 1980, pp. 327.

A.I.Fet, *Zhurnal fizicheskoi khimii* 55 (1981), 622 [in Russian].

A.I. Fet, "*The System of elements from the group-theoretic viepoint*,", in: Ray Hefferlin, *Periodic Systems and their Relations to the Systematic analysis of molecular data*, pp. 41–86. The Edwin Mellen Press, Lewiston, NY,1989.

V.A. Fock, *Izvestiia AN SSSR, Department of Mathematical and Natural Scieces*, 1935, № 2, 169 [in Russian].

V. Fock, *Zs; fur Physik* 98 (1936), 145.

M.N. Gaysinsky, *Centenary of the periodic table of chemical elements*, *Nauka*, Moscow, 1969 [in Russian].

M. Gell-Mann, *Phys. Rev.* 125 (1962), 1067.

F. Gürsey, L.A. Radicati, *Phys. Rev. Lett.* 13 (1964), 173.

R. Hefferlin, R. Campbell, H. Kuhlman, "*The periodic table of diatomic molecules. I.II.*", *J. Quant. Spectrosc. Rad. Transfer* 21 (1979), 315–336, 337–354.

R. Hefferlin, H. Kuhlman, "*The periodic system for free diatomic molecules.III*", *J. Quant. Spectrosc. Rad. Transfer* 24 (1980), 379–383.

B.G. Konopelchenko , *Preprint of the Institute of Nuclear Physics SB AS USSR*, *Novosibirsk*, 1972 [in Russian].

L.D. Landau, E.M. Lifshitz, "*Quantum mechanics*", Nauka, Moscow, 1972, pp. 368 [in Russian].

E. Madelung, "*Die mathematischen Hilfsmittel des Physikers*", Springer Verlag, Berlin, 1964.

I.A. Malkin, V.I. Man'ko, *JETP Letters* 2 (1965), 230 [in Russian].

A. Messiah, "*Quantum Mechanics Volume I, II*". North Holland Publishing Company, 1967.

Y. Néeman, *Nucl. Phys.* 26 (1961), 222.

S. Okubo, *Progr.Theor.Phys.* 27 (1962), 949.

A. Pais, *Phys. Rev. Lett.* 13 (1964), 175.

W. Pauli, "*Wave mechanics*", Dover Publications, 2000.

R. Refferlin, M. Kutzner, "*Systematics of ground-state potential minima between two main-group atoms of ions*", J. Chem. Phys. 75 (1981), 1035–1036.

Y.B. Rumer, A.I. Fet, "*The theory of unitary symmetry*", Nauka, Moscow. 1970, pp. 400 [in Russian].

Y.B. Rumer and A.I. Fet, *Teoreticheskaya i Matematicheskaya Fizika*, 1971, 9, p. 203 [in Russian].

Y.B. Rumer, A.I. Fet, "*Group theory and quantum fields*", Nauka, Moscow, 1977, pp. 247 [in Russian].

G. Seaborg, *Centenary of the periodic table of chemical elements,* Nauka, Moscow, 1969.

A. Sommerfeld, "*Atomic Structure and Spectral Lines*", Methuen & Co. Ltd. 1923.

N. Vilenkin, "*Special functions and the theory of group representations*", Nauka, Moscow, 1965, pp. 588 [in Russian].
E.P. Wigner, *Phys. Rev*. 40 (1932), 749.
E.P. Wigner, *Ann. Math*. 38 (1939).
E.P. Wigner, "*Group Theory and its Application to the Quantum Mechanics of Atomic Spectra*". *New York*: Academic Press, 1959.
T. Yao, *J. Math. Phys. I*, 1967, 8, 1931; II, 1968, 9, 1615.
G.V. Zhuvikin, R. Hefferlin, *Herald of the Leningrad State University*, 1983, issue 16, № 3, p. 10 [in Russian].

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