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 $\psi$ 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, $\psi$ 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 $\psi$ is defined for the given state with an accuracy up to a nonzero imaginary factor $\lambda$, so that $\psi$ 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:

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

where $d^3x = dx\,dy\,dz$, 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” $\psi$ (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 $\varphi$ is real and does not depend on the coordinates. The phase factor does not change the meaning of $\psi$, since all numerical values derived from the quantum theory do not depend on it. For the normalized wave function $\psi$, the probability of finding the particle in $D$ is

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

It can be shown that all quadratically integrable $\psi$ 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, $\psi$ 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

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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 $\psi$ into state $\varphi$. The probability of such transition is $|\langle \psi | \varphi \rangle|^2$, where

$$
\langle \psi | \varphi \rangle = \int \psi^*(x, y, z) \varphi(x, y, z) dx^3
$$

This expression is called the scalar product of the wave functions $\psi$ and $\varphi$; 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 $\psi$ is defined as the square root of the integral (1.1). The norm is used to define the convergence of series: a series $\cdots \psi_1 + \psi_2 + \cdots + \psi_n + \cdots$ is said to converge to $\psi_0$, if the norm $\psi_0 - s_n$ of its partial sum $s_n = \psi_1 + \cdots + \psi_n$ 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 $\psi$ and $\psi'$ 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 $\psi(x, y, z) dx^3$. 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 $\psi'(x', y', z') dx'^3$.

Since the situations are equivalent, the following probabilities coincide:

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

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

$$
|\psi'(x', y', z')| = |\psi(x, y, z)| \quad (1.5)
$$

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

$$
\psi'(x', y', z') = \psi(x, y, z) \quad (1.6)
$$

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

$$
|\langle \psi | \varphi \rangle|^2 = \left| \int \psi^*(x, y, z) \varphi(x, y, z) dx^3 \right|^2 = \left| \int \psi^*(x', y', z') \varphi'(x', y', z') dx'^3 \right|^2 = |\langle \psi' | \varphi' \rangle|^2 \quad (1.7)
$$

From eq. (1.7), it can be mathematically deduced that $\psi'(x', y', z') = e^{i\alpha} \psi(x, y, z)$ where the phase factor may depend on $\psi$, 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 \(O = (o_{ij})\):

\[
\begin{align*}
x' &= o_{11}x + o_{12}y + o_{13}z \\
y' &= o_{21}x + o_{22}y + o_{23}z \\
z' &= o_{31}x + o_{32}y + o_{33}z
\end{align*}
\]

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 \(\psi'\) directly through \(x, y, z\), apply the reverse rotation \(O^{-1}\) and replace \(x\) in eq. (1.8) by \(O^{-1}x\):

\[
\psi'(x) = \psi(O^{-1}x)
\]

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

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

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 \(\psi\) functions:

\[
\psi' = T_O \psi
\]

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 \( g_1 g_2 \) defined on \( G \) and \( \gamma \) the association law \( (g_1 g_2)g_3 = g_1(g_2 g_3) \), 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: \( T_1 T_2 \) designates the operator obtained as the result of the operator \( T_2 \) and then operator \( T_1 \), so

\[
T_3 = T_1 T_2 \text{ means that if } T_2 a = b, \ T_1 b = c, \text{ then } T_3 a = c
\]

(1.12)

Associative law for multiplication of operators is satisfied automatically, since the action of \( T_3 \) followed by \( T_1 T_2 \) means the same as the action of \( T_2 T_3 \) 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

\[
T \cdot 1 = 1 \cdot T = T.
\]

(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 \( SO(3) \). Henceforth, when talking about rotations, we mean proper rotations only.

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

\[
T_{O_2} \psi = \psi', \text{ where } \psi'(x) = \psi(O_1^{-1} x), \quad T_{O_1} \psi' = \psi'', \text{ where } \psi''(x) = \psi'(O_2^{-1} x)
\]

(1.14)

Substituting \( O_1^{-1} x \) instead of \( x \) in the definition of \( \psi' \), obtain

\[
\psi'(O_1^{-1} x) = \psi(O_2^{-1}(O_1^{-1} x)) = \psi(O_2^{-1} O_1^{-1} x) = \psi((O_1 O_2)^{-1} x),
\]

2 Spécial orthogonal.
and from the definition of $\psi''$

$$\psi''(x) = \psi(O^{-1}x)$$  \hfill (1.15)

Equation (1.15) means that successive application of operators $T_{o_2}$ and $T_{o_1}$ to the function $\psi''$ is equivalent to a single application of operator $T_{o_3}$; in other words,

$$T_{o_1}T_{o_2} = T_{o_3}$$  \hfill (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), $O_i^{-1}$ instead of $O_i$, obtain $T_oT_{o^{-1}} = 1$. Therefore, $T_{o^{-1}}$ is inverse to $T_o$:

$$T_o^{-1} = (T_o)^{-1}$$  \hfill (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

$$T_{g_1}T_{g_2} = T_{g_3}, T_e = 1,$$  \hfill (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:

$$T(\psi_1 + \psi_2) = T\psi_1 + T\psi_2, \quad T(\lambda \psi) = \lambda T\psi$$  \hfill (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, $T_0\psi_1 + T_0\psi_2 = T_0(\psi_1 + \psi_2)$. 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:

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

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

$$\langle \psi'|\varphi' \rangle = \int \psi'(x)\varphi'(x)dx = \int \psi'(O^{-1}x)\varphi(O^{-1}x)d^3x.$$
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 $\{Tg\}$ of a group $G$ is unitary, if operators $Tg$ 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

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

This operator commutes with all operators of rotation $T_O$,

$$T_O H = HT_O, \quad (1.22)$$

that is, both products are identical; in other words, for any function $\psi$, 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 $p^i$ and $V$. Let $T_O \psi = \psi'$. Then from eq. (1.10), we have

$$p^i \psi' = \frac{\hbar}{i} \frac{\partial}{\partial x} \psi' = \frac{\hbar}{i} \left( a_{ii} \frac{\partial \psi}{\partial x} + a_{ij} \frac{\partial \psi}{\partial y} + a_{ik} \frac{\partial \psi}{\partial z} \right), \quad (1.23)$$

and similarly for $p^j$ and $p^k$. 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 $\psi$ be an eigenfunction of the energy operator, that is, $H\psi = E\psi$. In this case, all functions $\psi' = T_O \psi$ obtained from $\psi$ by rotations are also eigenfunctions of $H$ with the same eigenvalues $E$. This is to be expected from symmetry reasons since states $\psi$ and $\psi'$ 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:

$$H\psi' = HT_O \psi = T_O H\psi = T_O (E\psi) = ET_O \psi = E\psi' \quad (1.24)$$

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 $\psi_0$; 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:
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 $\{T_0\}$ 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 $\varphi$ 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 $\{T_0\}$ 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:

$$T_0(c_1 \psi_1 + \ldots + c_k \psi_k) = T_0(c_1 T_0 \psi_1 + \ldots + c_k T_0 \psi_k) = c_1 T_0 T_0 \psi_1 + \ldots + c_k T_0 T_0 \psi_k$$

$$= c_1 T_0 T_0 \psi_1 + \ldots + c_k T_0 T_0 \psi_k$$

But $T_0 \psi_0$ are expressed in terms of $\psi_1, \ldots, \psi_k$, which are the basis for all functions $T_0 \psi_0$, so the right-hand side can be represented in the same form (eq. (1.25)). We denote this subspace $W_{\psi_0}$. Evidently, $W_{\psi_0}$ 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 $\{T_0\}$; 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 $W_{\psi_0}$ is also irreducible and $W_E = W_{\psi_0}$. Therefore, in the general case, eigenspaces of a spherically symmetric energy operator can be obtained simply by applying rotation operators $T_0$ to some eigenfunction and then by constructing linear combinations of these new eigenfunctions. From the dimension of space $W_{\psi_0}$, 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,

$$H = H_0 + H_1, \text{ where } H_0 = \frac{1}{2m} p^2 - \frac{Ze^2}{r} \text{ and } H_1 = V(r), \quad (1.27)$$
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 $\mathbb{R}$. 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 $\mathbb{R}$ a complete orthonormal basis of eigenfunctions of operator $H$, as it is done in the textbooks on quantum mechanics,

$$\psi_{n l m}(x, y, z) = f_n(r)Y_l^m(\varphi, \varphi),$$

(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 $-l$, $-l + 1, \ldots, l - 1, l$. “Radial functions” $f_n(r)$ decrease exponentially when $r \to \infty$, and $Y_l^m(\varphi, \varphi)$ are spherical functions defined on the sphere $S^2(x^2 + y^2 + z^2 = 1)$.

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

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

(1.29)

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

$$\psi = \sum_{n, l} \psi_{n l},$$

(1.30)

with orthogonal terms, where $\psi_{n l}$ are eigenfunctions of $H$ connected to eigenvalues $E_{n l}$, that is, they belong to the eigensubspace $W_{E_{n l}}$. Therefore, eq. (1.30) defines the expansion of the space of all wave functions $\mathbb{R}$ into the orthogonol sum of irreducible invariant subspaces of $SO(3)$ group (denoted, for brevity, $R_{n l}$):

$$\mathbb{R} = \bigoplus R_{n l}.$$  

(1.31)

Basis $R_{n l}$ 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 $m = -l$, $-l + 1, \ldots, l - 1, l$. 

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

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

(1.32)

and

$$R = R_1 \oplus R_2 \oplus \cdots \oplus R_n \oplus \cdots$$

(1.33)

**Table 1.1: Expansion of $R$ into irreducible subspaces.**

<table>
<thead>
<tr>
<th>$n = 1$</th>
<th>$n = 2$</th>
<th>$n = 3$</th>
<th>$n = 4$</th>
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<tr>
<td>$l = 0$</td>
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<tr>
<td>$\Psi_{4,1,-1}$</td>
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<td>$l = 2$</td>
<td>$\Psi_{3,2,0}$</td>
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<td>$m = 3$</td>
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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

$$R_n = R_{n0} \oplus \cdots \oplus R_{n,n-1}$$  

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

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

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 eigensubspace of $H$.

Expansion of $R$ into irreducible subspaces is conveniently represented by the following table, where the cells correspond to the basis functions $\psi_{nlm}$ (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 $T_O$ 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 $Ze$, eigenfunctions and eigenvalues of the energy operator $H_0$ are defined by the equation

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

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

$$E_n = -\frac{Ze^2}{2\hbar^2} \frac{1}{n^2}$$  

As mentioned in Section 1.1, eigenfunctions $\psi_{nlm}$ 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 $E_{n_l}(l = 0, 1, \ldots, n - 1)$ 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 $\tilde{\psi}(p_x, p_y, p_z)$ related to $\psi(x, y, z)$ by Fourier transform:

$$\tilde{\psi}(p_x, p_y, p_z) = (2\pi\hbar)^{-3/2} \int \psi(x, y, z)e^{-i(p_x x + p_y y + p_z z)/\hbar} dx,$$

$$\psi(x, y, z) = (2\pi\hbar)^{-3/2} \int \tilde{\psi}(p_x, p_y, p_z)e^{i(p_x x + p_y y + p_z z)/\hbar} dp.$$

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

$$\tilde{\psi} = U\psi, \quad \psi = U^{-1}\tilde{\psi}.$$  

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

$$\langle \tilde{\psi} | \tilde{\varphi} \rangle = \langle \psi | \varphi \rangle.$$  

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 $\tilde{R}$ of functions $\tilde{\psi}(p_x, p_y, p_z)$ (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,

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

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 $\tilde{R}_n = UR_n$ composed of eigenfunctions of eq. (1.41) associated with eigenvalues $E_n$ are orthogonal to each other and have the same dimension $n^3$.

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

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

$$\xi_1^2 + \xi_2^2 + \xi_3^2 + \xi_4^2 = 1$$

of a four-dimensional Euclidean space $R^4$ with distances between its points:
\[ |\xi - \eta| = \sqrt{[(\xi_1 - \eta_1)^2 + (\xi_2 - \eta_2)^2 + (\xi_3 - \eta_3)^2 + (\xi_4 - \eta_4)^2]}^{1/2} \]  

(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 \( \xi_n \) 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

\[ p_0 = \sqrt{-2mE} \]

(1.44)

is positive (and equals the mean square of the momentum \( p^2 \) in the state \( \tilde{\psi}(p) \)). 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:

\[
\begin{align*}
\xi_1 & = \frac{2p_0p_x}{p^2 + p_0^2} = \sin \alpha \sin \vartheta \cos \varphi \\
\xi_2 & = \frac{2p_0p_y}{p^2 + p_0^2} = \sin \alpha \sin \vartheta \sin \varphi \\
\xi_3 & = \frac{2p_0p_z}{p^2 + p_0^2} = \sin \alpha \cos \vartheta \\
\xi_4 & = \frac{p^2 - p_0^2}{p^2 + p_0^2} = \cos \alpha
\end{align*}
\]

(1.45)

where \( \alpha, \vartheta, \) and \( \varphi \) are the spherical coordinates on \( S^3 \) similar to usual coordinates \( \vartheta \) and \( \varphi \) on \( S^3 (0 \leq \alpha \leq \pi, 0 \leq \vartheta \leq \pi, 0 \leq \varphi \leq 2\pi) \). 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 \( \tilde{\psi}(p) \) of eq. (1.41) and the functions on the three-dimensional sphere is defined as follows:

\[ \Psi(\alpha, \vartheta, \varphi) = \frac{\pi}{\sqrt{8}} p_0^{5/2} (p^2 + p_0^2)^3 \tilde{\psi}(p), \]

(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 \( \tilde{\psi}(p) \) can be rewritten as the integral for \( \Psi \):

\[ \Psi(\alpha, \vartheta, \varphi) = \frac{\lambda}{2\pi^2} \int \Psi(\alpha', \vartheta', \varphi') d\Omega', \]

(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
\[
\lambda = \frac{Zme^2}{\hbar \sqrt{-2mE}}
\]  

(1.48)

Let \( E = E_n \). Then \( \psi \) belongs to the subspace \( \mathbb{R}^n \), 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

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

(1.49)

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

\[
\langle \Psi | \Phi \rangle = \langle \widetilde{\psi} | \widetilde{\phi} \rangle
\]

(1.50)

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

\[
\Psi = F_n \psi,
\]

(1.51)

which is linear, preserves scalar products, and transforms the space of eigenfunctions \( \mathbb{R}^n \) 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 \( \mathbb{R}^n \) and \( F_n \).

Space \( F_n \) is very simple to describe. It consists of four-dimensional spherical functions of order \( n \). 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:

\[
\Delta u_l(x, y, z) = 0
\]

(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 \( l \)” \( Y_l(\vartheta, \varphi) \). 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 \( \text{SO}(3) \) 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 \(Y_\theta (\vartheta, \varphi)\). Each of the basic spherical functions \(Y_l^m(\theta, \varphi)\) 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 wavefunctions \(\psi_{n}\)(\(x, y, z\)) = \(f_n(r)Y_l(\theta, \varphi)\), 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 \(\psi_{nl}\) (eqs. (1.30) and (1.31)), the rotation group acts in the same way as in the space of spherical functions \(Y_r\). 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:

\[
\Delta^{(4)}u_n = \frac{\partial^2 u_n}{\partial \xi_1^2} + \frac{\partial^2 u_n}{\partial \xi_2^2} + \frac{\partial^2 u_n}{\partial \xi_3^2} + \frac{\partial^2 u_n}{\partial \xi_4^2} = 0
\]  

(1.53)

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

\[
\Psi_{nlm}(\alpha, \theta, \varphi) = \Pi_n(\alpha)Y_l^m(\theta, \varphi)
\]  

(1.54)

where \(Y_l^m(\theta, \varphi)\) are ordinary spherical functions \((m = -l, -l+1, \ldots, l-1, l)\), and \(l\) takes values 0, 1,..., \(n - 1\). The Fock transform carries the eigenfunctions \(\psi_{nlm}(x, y, z)\) of the Schrödinger equation into four-dimensional spherical functions \(\Psi_{nlm}(\alpha, \theta, \varphi)\) 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 \(Y_{n-1}(\alpha, \theta, \varphi)\). In particular, the basis for these functions consists of the above functions \(\Psi_{nlm}\). 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 \(R_{nl}\) 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 \(F_n\) \((n = 1, 2,...)\) a single transform \(F\) of the space of all wave functions \(\mathbb{R}\) into the space of all square-integrable functions on the sphere \(S^3\); this Hilbert space is denoted as \(\mathbb{F}\) 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 $\mathbb{R}^n$, so that $F\psi_{nlm} = \Psi_{nlm}$; for wave functions which are not eigenfunctions of $H_0$, use eq. (1.32) and define

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

(1.55)

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

$$\langle F\psi | F\varphi \rangle = \left( \sum_n F_n \psi_n \sum_n F_n \psi_n' \right) = \sum_n \langle F_n \psi_n | F_n \varphi_n \rangle$$

(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

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

(1.57)

and, therefore, can be obtained by $F$ from function

$$\psi = \sum_{n=1}^{\infty} F^{-1}_n(\Psi_{n-1})$$

(1.58)

Thus, operator $F$ defines an isomorphism of the Hilbert space $\mathbb{R}$ of Schrödinger wave functions on the Hilbert space $\mathbb{F}$ 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 $\text{SO}(4)$, greater than the rotation group of three-dimensional space $\text{SO}(3)$, naturally acts on the space $\mathbb{F}$.

### 1.3 Broken symmetry

Consider a rotation group in the four-dimensional Euclidean space $\mathbb{R}^4$ with coordinates $\xi_1, \xi_2, \xi_3, \xi_4$. This is a group of homogeneous linear transforms preserving distances and written similar to eq. (1.8):

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

(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 $\det|O| = +1$.

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

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

or

$$\Psi'(\xi_1, \xi_2, \xi_3, \xi_4) = \Psi(o_{11}\xi_1 + \cdots + o_{1n}\xi_n, \cdots, o_{41}\xi_1 + \cdots + o_{4n}\xi_n)$$  \hspace{1cm} (1.61)

Just as three-dimensional rotations, operators

$$\Psi' = T_0\Psi$$  \hspace{1cm} (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 $T_0$ 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

$$\langle \Psi'|\Phi' \rangle = \int \Psi''(\xi')\Phi'(\xi')d\Omega' = \int \Psi'(O^{-1}\xi)\Phi(O^{-1}\xi)d\Omega .$$  \hspace{1cm} (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 $T_0 \{ \}$ 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 $e_k \rightarrow e'_k$, 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:

\[
\begin{array}{ccc}
R & \xrightarrow{T} & R \\
W & \downarrow & W \\
R' & \xrightarrow{T'} & R'
\end{array}
\]  \hspace{1cm} (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

\[
T' = WTW^{-1}
\]  \hspace{1cm} (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

\[
T'_g = WTW^{-1}
\]  \hspace{1cm} (1.66)

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

\[
T_g = W^{-1}T'_g W
\]  \hspace{1cm} (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.\footnote{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.}

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...
$\mathbb{F}_n$ (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 $\tilde{\psi}(p)$ (eq. (1.38)), and $\psi'(x)$ to $\tilde{\psi}'(p)$. Then the operator $T_O$ corresponds in the momentum space to the operator which carries $\tilde{\psi}(p)$ into $\tilde{\psi}'(p)$.

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

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

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

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

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,

$$\tilde{\psi}'(p) = \tilde{\psi}(O^{-1}p)$$

(1.68)

and functions $\tilde{\psi}(p)$ 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 $\xi$ (defined by angles $\alpha, \beta, \varphi$) 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 $\mathbb{R}_n$; then $E = E_0$ and $p_0 = \sqrt{-2mE_0}$ (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 $\xi, (\xi' = \xi)$ and $\xi_1, \xi_2, \xi_3$ are transformed by the same matrix $O^{-1}$ as $p_1, p_2, p_3$; so we have

$$\begin{align*}
\xi'_1 &= o_{11}^\dagger \xi_1 + o_{12}^\dagger \xi_2 + o_{13}^\dagger \xi_3 \\
\xi'_2 &= o_{21}^\dagger \xi_1 + o_{22}^\dagger \xi_2 + o_{23}^\dagger \xi_3 \\
\xi'_3 &= o_{31}^\dagger \xi_1 + o_{32}^\dagger \xi_2 + o_{33}^\dagger \xi_3 \\
\xi'_4 &= \xi_4
\end{align*}$$

(1.69)

Since the factor of $\tilde{\psi}(p)$ 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 $\xi'$ is defined by eq. (1.69). The transform eq. (1.69) is inverse to the special four-dimensional rotation with matrix
Thus, in view of the Fock equivalence, the operator $T_0$ in space $\mathbb{R}$ corresponds to the operator carrying $\Psi(\xi')$ into

$$\Psi''(\xi') = \Psi(\xi') = \Psi(O^{-1}_4 \xi')$$

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 $\xi_4$, that is, $\xi_4' = \xi_4$. All such rotations constitute a subgroup of $\text{SO}(4)$, 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 $\text{SO}(3)$ and will be denoted simply $\text{SO}(3)$. Therefore, *Fock equivalence carries the representation (1.9) of group $\text{SO}(3)$ 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 $\text{SO}(3)$ 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 $\text{SO}(4)$ 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 $\text{SO}(4)$:

$$F = F_1 \oplus F_2 \oplus \cdots \oplus F_n \oplus \cdots$$

Decomposition (1.34) corresponds to the decomposition of $F_n$ in terms of *irreducible subspaces* of $\text{SO}(3)$:

$$F_n = F_{n,0} \oplus F_{n,1} \oplus \cdots \oplus F_{n,n-1},$$

where $F_{n,l}$ is the image of space $\mathbb{R}_{nl}$ 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:

$$\Psi(\xi) = \sum_{n,l,m} c_{nlm} \psi_{nlm}(\xi')$$

Subspaces $F_n$ are invariant even for the whole group $\text{SO}(4)$. 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 $\psi_{nlm}$ in Table 1.1 are changed for corresponding vectors $\Psi_{nlm}$, 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) ($\xi_4$ 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 whether 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, 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 $C$,

\[
\begin{align*}
\xi_1' &= c_{11} \xi_1 + \cdots + c_{16} \xi_6 \\
\cdots & \quad \cdots \\
\xi_6' &= c_{61} \xi_1 + \cdots + c_{66} \xi_6
\end{align*}
\]  

(1.75)

having determinant +1 and preserving the form

\[
\xi_1^2 + \xi_2^2 + \xi_3^2 + \xi_4^2 - \xi_5^2 - \xi_6^2
\]

(1.76)

That is,\(^8\)

\(^8\) 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).
1.3 Broken symmetry

\[ \xi'^2 + \xi'^2 + \xi'^2 + \xi'^2 - \xi'^2 = \xi_1^2 + \xi_2^2 + \xi_3^2 - \xi_4^2. \]  

(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 \( \xi_5, \xi_6 \), that is, \( \xi'_5 = \xi_5, \xi'_6 = \xi_6 \), and from eq. (1.77), we have

\[ \xi'^2 + \xi'^2 + \xi'^2 + \xi'^2 = \xi_1^2 + \xi_2^2 + \xi_3^2 + \xi_4^2. \]  

(1.78)

Identified with the coordinates of the four-dimensional Euclidean space, the first four coordinates \( \xi_n \) can be regarded as four-dimensional rotations with matrices:

\[ C = \begin{bmatrix}
  o_{11} & \cdots & o_{14} \\
  \vdots & \ddots & \vdots \\
  o_{41} & \cdots & o_{44}
\end{bmatrix}, \]  

(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 \( R_{n\ell} \) (instead of \( F_{n\ell} \)) 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 \( \psi \) from \( R_n \) and any operator of a four-dimensional rotation \( T_{o\ell} \), we have \( T_{o\ell} H_0 \psi = T_{o\ell} (E_n \psi) = E_n T_{o\ell} \psi = H_0 (T_{o\ell} \psi) \), and from eq. (1.32) \( T_{o\ell} H_0 \psi = H_0 T_{o\ell} \psi \).
for all $\psi$ from $\mathbb{R}$. But for the group $\text{SO}(4,2)$, we can no longer find a Hamiltonian to commute with the group; since the whole space $\mathbb{R}$ is irreducible for this group, such Hamiltonian would have the whole $\mathbb{R}$ as its eigenspace with a single eigenvalue. For this hypothetical Hamiltonian $H_*$, we would have

$$H_*\psi = E\psi$$  \hspace{1cm} (1.80)

Such an operator is sometimes called “constant.” Since energy is accurate within a constant, we can introduce a term $H_0$ in the Hamiltonian equation (1.27), so that $H_0$ 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 $H_1$ which does not commute with $\text{SO}(3)$; 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

$$H = H_* + H_0 + H_1 + H_2,$$  \hspace{1cm} (1.81)

where $H_*$ commutes with $\text{SO}(4,2)$, $H_0$ commutes with $\text{SO}(4)$, and $H_1$ commutes with $\text{SO}(3)$. 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 $\text{SO}(4,2)$; perturbation $H_0$ reduces the symmetry, so that $H_* + H_0$ has the symmetry of subgroup $\text{SO}(4)$; then the following perturbation $H_1$ reduces the symmetry to the subgroup $\text{SO}(3)$. The last term $H_2$ completely breaks the symmetry of the system.\footnote{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 eigenspaces are one-dimensional and not interesting as far as symmetry groups are considered.}

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:

$$\text{SO}(4,2) \supset \text{SO}(4) \supset \text{SO}(3)$$  \hspace{1cm} (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 $\text{SO}(4)$ ($n = 1, 2, \ldots$); all vectors with given $n$, $l$ generate an irreducible subspace $F_{nl} \subset F_n$ of subgroup $\text{SO}(3)$ ($l = 0, 1, \ldots, n - 1$); finally, the third index $m$, for given $n$, $l$ enumerates individual
basis vectors in $F_m(m = -l, -l + 1, \ldots, l - 1, l)$. 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 \textit{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.