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DEVELOPMENT OF THE BETHE METHOD FOR THE CONSTRUCTION OF TWO-VALUED SPACE GROUP REPRESENTATIONS AND TWO-VALUED PROJECTIVE REPRESENTATIONS OF POINT GROUPS

A procedure of calculation of two-valued space group representations and two-valued projective representations of point groups is considered. A method of construction of factor systems $\omega_2(r_2, r_1)$, which reflect the transformations of half-integer spin quantum wave functions and are required in order to find the two-valued irreducible projective representations of the point groups, is presented. This method is based on the introduction of an operation q, firstly used by Bethe, as an additional symmetry element. The pathway of introducing the relations, which permit to make a one-valued algebra of double groups and, particularly, their multiplication tables, is shown by the examples of the 222 (D_2) and 32 (D_3) groups. The construction of a standard factor-system $\omega'_{(1)}(r_2, r_1)$ of the projective class K_1 for the group 222 on the base of the discussed relations is presented for the first time. The whole role and the possibilities of Bethe's method and its modifications for the construction of two-valued representations of the point and space groups are discussed.

Keywords: Bethe's method, two-valued space group representations, two-valued projective representations of point groups.

Finding the spinor representations of space symmetry groups is required for solving a wide range of crystal spectroscopy problems, in particular, the spectroscopy of zones-indirect or indirect semiconductors, with absolute extremes of electronic bands, i.e. absolute maximum of the valence band and absolute minimum of the conduction band located at the different points of the Brillouin zone. These representations allow fulfilling the classification of the electronic states of crystals at any points of the Brillouin zone, which is a basis, in its turn, for the classification of their exciton states, which are often investigated by using spectroscopy methods.

The irreducible representations of full space groups $\mathbf{D}_{\{\mathbf{k}\}}$ possessing the irreducible star $\{\mathbf{k}\}$ are determined through the representations of the groups of the wave vectors $\mathbf{D}_{\mathbf{k}}$, which are also called the small representations. The general method of construction of irreducible representations $\mathbf{D}_{\mathbf{k}}$ of the groups of the wave vectors $G_{\mathbf{k}}$, including spinor, in the form of the projective representations of point groups of equivalent directions $F_{\mathbf{k}}$ of the groups of the wave vectors, which are isomorphic to the factor-groups of the group $G_{\mathbf{k}}$ on the infinite invariant subgroup of translations, is presented in [1].

We recall that the projective representations or ray representations satisfy the relations

$$\mathbf{D}(r_2)\mathbf{D}(r_1) = \omega(r_2, r_1)\mathbf{D}(r_2 r_1), \tag{1}$$

where the set of numbers $\omega(r_2, r_1)$ named a factor-system possesses the property

$$|\omega(r_2, r_1)| = 1. \quad (2)$$

The irreducible representations of the wave vector group $\mathbf{D_k}$ contain the infinite number of members $\mathbf{D_k}(h)$ for the elements $h \in G_\mathbf{k}$. Each element h can be presented as $h = (\boldsymbol{\alpha} + \mathbf{a}|r)$, where r – "rotational" element, the aggregate of which forms the point group $F_\mathbf{k}$, $\boldsymbol{\alpha}$ is the vector of a nontrivial translation corresponding to a rotational element r, and $\mathbf{a}$ is the vector of a trivial translation on the periods of the Bravais lattice.

The values of matrices $\mathbf{D_k}(h)$ and their characters $\chi_{\mathbf{D_k}(h)}$ are given by the formulas

$$\mathbf{D_k}(h) = e^{-ik(\alpha+a)} w(r)\mathbf{D}(r) \quad (3)$$

and

$$\chi_{\mathbf{D_k}(h)} = e^{-ik(\alpha+a)} w(r)\chi_{\mathbf{D}(r)}, \quad (4)$$

where for representations describing the state without taking the spin into account (with integer spin), $w(r) = u(r) \equiv u_1(r)$ is the function, which brings the factor-system $\omega(r_2, r_1) \equiv \omega_1(r_2, r_1)$, which is determined by the properties of the crystal spatial group, to the standard form $\omega'(r_2, r_1) \equiv \omega'_1(r_2, r_1)$; for representations, describing the states involving the spin (with a half-integer spin), $w(r) = u_s(r) = u_1(r)u_2(r)$ is the function, which brings the factor-system $\omega(r_2, r_1) = \omega_s(r_2, r_1) = \omega_1(r_2, r_1)\omega_2(r_2, r_1)$, which is determined by the transformations of spinors in the spatial group, to the standard form $\omega'(r_2, r_1) = \omega'_s(r_2, r_1) = \omega'_1(r_2, r_1)\omega'_2(r_2, r_1)$; $u_2(r)$ is the function, which brings the factor-system $\omega_2(r_2, r_1)$, which is determined by the transformations of spinors at the operations of symmetry of groups of directions of groups of the wave vector $F_\mathbf{k}$, to the standard form $\omega'_2(r_2, r_1)$; $\mathbf{D}(r)$ – corresponding to the standard factor-system the irreducible projective representations of that class, which the factor-system $\omega(r_2, r_1)$ (as a rule, these classes are K_0 and K_1) belongs to, and $\chi_{\mathbf{D}(r)}$ are characters of the irreducible projective representations $\mathbf{D}(r)$.

The construction of a factor-system $\omega_1(r_2, r_1)$ is performed by the formula

$$\omega_1(r_2, r_1) = e^{i(\mathbf{k} - r_2^{-1}\mathbf{k})\boldsymbol{\alpha}_1} \quad (5)$$

and, for any point of the Brillouin zone, does not cause any difficulties. It is easy to define the class, to which this factor-system belongs [1].

The factor-system $\omega_2(r_2, r_1)$ is determined by the condition

$$\omega_2(r_2, r_1) = \begin{cases} 1 & \text{at } 0 \leqslant \vartheta < 2\pi, \\ -1 & \text{at } 2\pi \leqslant \vartheta < 4\pi, \end{cases} \quad (6)$$

where ϑ is a rotation angle corresponding to the composition of elements $r_2 r_1$. The class, to which it belongs, can be also easy set [1].

There is a particular interest in the case where both factor-systems $\omega_1(r_2, r_1)$ and $\omega_2(r_2, r_1)$ belong to the class K_1, i.e., when $K^{(1)} = K_1$ and $K^{(2)} = K_1$, where the numerical indices in brackets indicate the types of factor-system. In this case, the factor-system $\omega_s(r_2, r_1)$, as a composition of classes determined by the relations $K_0^2 = K_0$, $K_0K_1 = K_1K_0 = K_1$, and $K_1^2 = K_0$, belongs to the class K_0, and the representations describing the states taking the spin into account (half-integer spin) are projectively equivalent (p-equivalent) to a general vectorial, and representations describing the states without taking the spin into account (with integer spin) are p-equivalent to two-valued ones.

Thus, taking into account that the standard factor-system of the class K_0 completely consists of coefficients equal to 1, and matrices of representations corresponding to standard factor-systems, for the class K_0, where they coincide with ordinary vectorial, and for the class K_1, where they can be easily calculated, are known, the problem of construction of the irreducible representations of complete spatial groups and, in particular, the spinor ones, is reduced to the tasks of construction of the factor-system $\omega_2(r_2, r_1)$, determination of the form of standard factor-systems of the class K_1, and finding the functions $u_2(r)$ leading the factor-system $\omega_2(r_2, r_1)$ to the p-equivalent standard form.

We now describe the technique developed by us allowing, in the general and particular cases, to solve the above problems and thereby to build irreducible two-valued representations of point groups in the form of projective representations.

Bethe's method of construction of double point symmetry groups, which uses the operation q, is widely used for considering the symmetry of quantum systems with half-integer spin [2] (see, e.g., [3–5]). The operation q is a rotation by an angle of 2π around an arbitrary axis, which commutes with all other symmetry operations, acts on the wave function (spinor), determining the state of the quantum system, and changes its sign. The unit operation e is treated as a rotation around an arbitrary axis by an angle of 4π. Therefore, the equation $q^2 = e$ is fulfilled, which is the defining relation for the operation q.

The question of how the operator q is associated with the inversion i, which also commutes with all the operations of symmetry point groups, with reflection in an arbitrary plane σ and mirror rotation s_n around an axis of the n-th order, consisting of the rotation c_n and the reflection σ_h in a plane perpendicular to the axis of rotation, remains unclear.

Indeed, the usual definition of inversion operation is given by the formula $i \equiv s_2 = \sigma_h c_2$ [1], where c_2 is a rotation around the second-order axis, and σ_h – reflection in a plane perpendicular to this axis. It is assumed that the relation $\sigma_h = ic_2$ is met, and the relations $i^2 = e$ and $\sigma_h^2 = e$, which are defining for the operations of inversion and reflection, are also met. It is easy to see that, when considering the symmetry properties of quantum systems with half-integer spin within the Bethe method from the equation $i = \sigma_h c_2$ by substituting the above expression $\sigma_h = ic_2$, the relation $i = ic_2c_2$, i.e. $i = iq$, or $i = qi$ follows, which is apparently wrong.

The authors are unaware of any attempts in the literature to overcome the above-mentioned difficulty, and this attempt is made in the present publication.

The aim is to reasonably introduce the operation q into the group containing operations i, σ. and s_n [2]. This could be achieved, in general, in two ways.

The first way is to preserve the same definition of inversion for the double groups as for the ordinary ones

$$i = \sigma_h c_2.$$

This way leads to a change in the definition of reflection operation in the double groups. Indeed, by multiplying the equality $i = \sigma_h c_2$ by c_2 on the right, we can find that $ic_2 = \sigma_h c_2 c_2$, i.e. $ic_2 = \sigma_h q$ or $\sigma_h = qic_2$. Thus, the following equations is noncontradictory for the double groups:

$$i = \sigma_h c_2 \quad \text{and} \quad \sigma_h = qic_2. \tag{7}$$

The second way is to preserve the same definition of reflection for the double groups as for the ordinary ones:

$$\sigma_h = ic_2.$$

This way leads to a change in the definition of inversion operation for the double groups. Indeed, by multiplying the equality $\sigma_h = ic_2$ by c_2 on the right, we can find that $\sigma_h c_2 = ic_2c_2$, i.e. $\sigma_h c_2 = iq$ or $i = q\sigma_h c_2$. This means that the following equation is also noncontradictory for double groups:

$$i = q\sigma_h c_2 \quad \text{and} \quad \sigma_h = ic_2. \tag{8}$$

For the certainty, we have to choose one of the considered above cases.

In our opinion, from the two options (without any loss of generality), logically more preferable is the second one, in which the inversion operation more complex in interpretation for the double groups is overridden, and the operation of reflection retains the former definition. Equations (8) can be considered thus as postulating the definitions of the inversion and reflection operations in the double groups.

It should be noted that, in the above definition of inversion preserving the conventional definition of reflection for ordinary groups, inversion rotations, which, along with reflections in double groups should be chosen as the symmetry elements of the second type, cannot be, as in the ordinary groups, replaced by the mirror rotations, as the inversion rotations $ic_n = q\sigma_h c_2 c_n = qc_2\sigma_h c_n = qc_2 s_n$ (here, $i \neq s_2$, as $s_2 = \sigma_h c_2$, and $i = q\sigma_h c_2 = qs_2$) qualitatively differ from the mirror rotations s_n by the multiplication by the operation q.

In double groups, the defining relations (not to be confused with definitions) for the operations of inversion and reflection, which are expressed in conventional groups by the equalities $i^2 = e$ and $\sigma^2 = e$, are also changed. Here, regardless of two above-described ways to define the inversion and the reflection for both of these, there are two possible options.

It is easy to see that, for two above-mentioned ways to define the inversion and the reflection in the double

[1] Here and further, as usual, the operation standing on the right is performed first.

[2] Double groups are not the direct products of the ordinary groups, except containing only one element e of the trivial group 1 (C_1 or E), and the double group $1'(C_1'$ or $E')$ consisting of the elements e and q. This follows from the fact that, otherwise, no power of the elements of the ordinary group would not have to be equal to expanding the group element q, which, in this case, is not so.

groups, the equality $i^2 = q\sigma_h^2$ is fulfilled. This means that the defining relations for the inversion and the reflection can be written either in the form of

$$i^2 = e \quad \text{and} \quad \sigma_h^2 = q \quad (\sigma_h^4 = e), \tag{9}$$

where the defining relation for the inversion used in the ordinary groups is preserved, either in the form

$$\sigma_h^2 = e \quad \text{and} \quad i^2 = q \quad (i^4 = e), \tag{10}$$

where the defining relation for the reflection operation is preserved.

In our opinion, easier and more convenient (without loss of generality) are the defining relations expressed by the equations (9), in which the defining relations are similar for the operations i and q, which commute with all other elements of symmetry.

Thus, in general, there are four possibilities for the noncontradictory introduction of the operator q: 1) using Eqs. (7) and (9); 2) (7) and (10); 3) (8) and (9); and 4) (8) and (10). Here, in our opinion, we should be limited to the preferred choice defined by Eqs. (8) and (9), i.e., the relations

$$\begin{aligned} &i = q\sigma_h c_2 \,(\text{this yields } \sigma_h = ic_2), \\ &i^2 = e \,\left[\text{this yields } \sigma_h^2 = q\,(\sigma_h^4 = e)\right]. \end{aligned} \tag{11}$$

It is convenient to have namely relations (11) as a basis of the systematics of irreducible double-valued projective representations of point symmetry groups and the systematics of factor-systems of the classes K_0 and K_1 and the functions $u(r)$ bringing these factor-systems to the p-equivalent standard form.

Let us consider the way of how the q-operator is introduced into the groups containing several axes. This can be conveniently done by the examples of the groups 222 (D_2) and 32 (D_3).

Let us start with the group D_2, where the constituting elements are the elements $a = c_2(c_{2z})$ and $b = u_2(c_{2x})$. The group D_2 contains only 4 elements: e, c_2, u_2, and u_2'. It is natural that the defining relations $a^4 = e$ ($a^2 = q$) and $b^4 = e$ ($b^2 = q$) are valid for the constituting elements of the double group D_2'. Let us clarify the question of how the operator q is included into the commuting defining relation for the constituting elements of the group and how the element $u_2'(c_{2y})$ is related to the elements c_2, u_2, and q.

Let us find firstly the commuting defining relation for the constituting elements of the double group D_2'. For the ordinary group D_2, it has a form $ab = ba$.

Let us use the general relation for an infinite group of rotations K:

$$f^{-1}c_\ell(\alpha)f = c_{f^{-1}\ell}(\alpha), \tag{12}$$

where $c_\ell(\alpha)$ – rotation by angle α around the axis ℓ, and f – any rotation. The extension of this relation onto the elements of the double groups included into the double rotation group K' can obviously be done in two ways. The first one consists in postulating the feasibility of this relation for the elements of the double groups with the treatment of the unit operation like turning by 4π angle, and the second - in postulating, with the same interpretation of the unit operation, the feasibility of the relation

$$f^{-1}c_\ell(\alpha)f = c_{f^{-1}\ell}(\alpha + 2\pi). \tag{13}$$

Let us take as a postulate, as easier, the first case. This again does not lead to any loss of generality.

Considering c_2 as $c_\ell(\pi)$ ($\ell \parallel Oz$), assuming $f = qu_2 = qc_{\ell'}(\pi)$ ($\ell' \parallel Ox$), and taking into account that $f^{-1} = u_2 = c_{\ell'}(\pi)$, relation (12) for the double group yields $c_{\ell'}(\pi)c_\ell(\pi)qc_{\ell'}(\pi) = c_{f^{-1}\ell}(\pi)$. Considering also $f^{-1}\ell = c_{\ell'}(\pi)\ell = -\ell$, we can find $qc_{\ell'}(\pi)c_\ell(\pi)c_{\ell'}(\pi) = c_{-\ell}(\pi)$ [3]. As $c_{-\ell}(\pi) = qc_\ell(\pi)$, we obtain $qu_2c_2u_2 = qc_2$.

Multiplying this relation on the left by u_2, we obtain

$$c_2u_2 = qu_2c_2 \quad \text{or} \quad ab = qba, \tag{14}$$

which is a commuting defining relation for constituent elements of the double group D_2'. It is essential that the operation q is included into the commuting defining relation for the double group D_2', unlike for the ordinary group D_2.

The definition of the element u_2' in the double group D_2' can be also given on the basis of Eq. (12).

Indeed, the relation $c_4u_2qc_4^3 = u_2'$ given in agreement with relation (12) can be considered as the definition of the element u_2' in the double group D_2'. Here, $u_2 = c_\ell(\pi)$ ($\ell \parallel Ox$), $f = qc_4^3 = qc_{\ell'}(3\pi/2)$ ($\ell' \parallel Oz$),

[3] Here, we could also select $f = u_2 = c_{\ell'}(\pi)$ ($\ell' \parallel Ox$), and as it would follow $f^{-1} = qu_2 = qc_{\ell'}(\pi)$. This would lead to the same result, as, in this case, $f^{-1}\ell = qc_{\ell'}(\pi)\ell = -\ell$.

$f^{-1} = c_4 = c_{\ell'}(\pi/2)$, $f^{-1}\ell = c_{\ell'}(\pi/2)\ell = \ell''$ ($\ell'' \parallel O\mathbf{y}$), and $u_2' = c_{2\mathrm{y}} = c_{\ell''}(\pi)$.

From the same relation (12), we can obtain a commuting relation for the elements c_4 and u_2. Assuming $c_4 = c_\ell(\pi/2)$ ($\ell \parallel O\mathbf{z}$) and $f = qu_2 = qc_{\ell'}(\pi)$ ($\ell' \parallel Ox$) and taking into account that $f^{-1} = u_2 = c_{\ell'}(\pi)$ and $f^{-1}\ell = c_{\ell'}(\pi)\ell = -\ell$, we can obtain $c_{\ell'}(\pi)c_\ell(\pi/2)qc_{\ell'}(\pi) = c_{-\ell}(\pi/2)$. Since $c_{-\ell}(\pi/2) = qc_\ell(3\pi/2) = qc_\ell^3(\pi/2)$, we obtain $u_2c_4qu_2 = qc_4^3$ or $qu_2c_4u_2 = qc_4^3$. Multiplying this relation by u_2 on the left, we can obtain the relation $c_4u_2 = qu_2c_4^3$, which is commuting for the elements c_4 and u_2.

Using the commuting relation for the elements c_4 and u_2 from the relation $u_2' = qc_4u_2c_4^3$, which defines the element u_2', it is easy to show that $u_2' = qqu_2c_4^3c_4^3 = u_2c_4^6 = u_2c_2^3 = qu_2c_2 = qba$, i.e.

$$u_2' = qu_2c_2 \quad \text{or} \quad u_2' = qba. \tag{15}$$

It should be noted that the operation $c_4 = c_\ell(\pi/2)$ ($\ell \parallel O\mathrm{z}$) used for deriving the equation defining the element u_2' plays a supporting role. This operation does not belong to the group D_2, but it, as well as all the elements of this group, is one of the operations of the infinite group of rotations K, for all elements of the double symmetry group K' of which, the relation (12) is correct.

With the defining relations for constituting elements and relations (14) and (15), it is easy to find the factor-system $\omega_2(r_2, r_1)$, which is defined by relation (12) and describes the properties of spinors in the group D_2.

For example, the coefficient $\omega_2(c_2, u_2') = -1$ in the case $r_1 = u_2'$ and $r_2 = c_2$, since the product $r_2r_1 = c_2u_2' = a(qba) = qaba = q(ab)a = q(qba)a = ba^2 = qb = qu_2$ is the element, which differs from the element u_2 included into the group D_2 by the factor q, i.e. by the additional rotation by an angle of 2π [since the element q is the rotation by 2π angle around an arbitrary axis, in the expressions of the form $qc_\ell(\alpha)$ it can always be interpreted as an additional rotation around the same axis ℓ]. For example, the coefficient $\omega_2(u_2, c_2) = -1$ in the case $r_1 = c_2$ and $r_2 = u_2$, since, in this case, $r_2r_1 = u_2c_2 = ba = q(qba) = qu_2'$. Here, of course, for all intrinsic rotations included into the infinite group of rotations K, the values of angle ϑ are limited by $0 \leqslant \vartheta < 2\pi$. Generally, since we can choose either elements $c_\ell(\alpha)$ or elements $qc_\ell(\alpha)$ in the transition from double to ordinary groups as their intrinsic rotations from the elements of double groups, the difference between them in the ordinary groups disappears, every intrinsic rotation can be interpreted as the rotation by an angle of ϑ lying within the range determined by the inequality $0 \leqslant \vartheta < 2\pi$ or $2\pi \leqslant \vartheta < 4\pi$. Without loss of generality, however, for their intrinsic rotations in the ordinary groups, we may postulate the feasibility of only one of these inequalities. Preferring a simpler case, we postulate, as was already noted above, that, for all intrinsic rotations belonging to the infinite group of rotations K, the whole range of rotation angles ϑ is determined only by the inequality $0 \leqslant \vartheta < 2\pi$. It can be shown that this inequality holds for all nonintrinsic rotations, i.e. for all elements of the infinite full orthogonal group $K_h = K \times C_i$. Indeed, as follows from the introduced defining relation for the inversion (9) $\sigma_h^2 = q$, which means that, for the element σ_h in the double groups, we should ascribe a rotation by an angle of π or 3π around an arbitrary axis (this corresponds to the existence in the double group of two elements σ_h and $q\sigma_h$). Then the inversion operation itself, which is defined by Eq. (8), must be, in accordance with this definition, compared to the rotation depending on the angle of the element σ_h either by an angle equal to zero or by an angle of 2π (this also corresponds to the existence in double groups of two elements – i and qi). Since the difference between the elements i and qi disappears in the ordinary group, we can postulate, without loss of generality, that the rotation only by an angle equal to zero or 2π corresponds to the inversion operation. Again, preferring a simpler version, we postulate that the inversion operation corresponds to the rotation by an angle equal to zero. This means that, for all the nonintrinsic rotations and for all the elements of the infinite complete orthogonal group K_h, the entire range of the values of rotation angles ϑ is defined by the inequality $0 \leqslant \vartheta < 2\pi$.

It should be noted also that the possibility of matching the inversion operation and rotation by an angle equal to zero could be the basis for determining the choice of the inversion operation in binary groups and its defining relation. It is easy to see that this feature is available, when we made, on the basis of logical considerations, choice defined by relations (8) and (9).

The factor system $\omega_2(r_2, r_1)$, which was found for the group D_2 in the above-mentioned way, can be conveniently represented as a table

$$\begin{array}{cc|cccc}
\omega_2(r_2, r_1) & r_1 & & & & \\
r_2 & & e & c_2 & u_2 & u_2' \\
\hline
b^0a^0 & e & 1 & 1 & 1 & 1 \\
b^0a^1 & c_2 & 1 & -1 & 1 & -1 \\
b^1a^0 & u_2 & 1 & -1 & -1 & 1 \\
qb^1a^1 & u_2' & 1 & 1 & -1 & -1
\end{array} \tag{16}$$

(left column shows the way, in which the elements of symmetry in the double group D_2' are defined in terms of products of constituting elements in the corresponding powers and q-operator)

For each pair of the commuting elements r_1 and r_2 distinct from the unity in the group D_2 (there are three such pairs of elements in this group), for example, for the pair of elements $r_1 = a = c_2$ and $r_2 = b = u_2$, the relation $\frac{\omega_2(r_2, r_1)}{\omega_2(r_1, r_2)} = -1$ holds. This means that the factor system (16) belongs to the class K_1, and the group D_2 contains irreducible projective representations belonging to the class K_1.

The membership of the factor system (16) to the projective class K_1 could also be established by the value of constant α', which determines the projective class of the factor-system $\omega(r_2, r_1)$ and, according to [1], can be calculated for the groups D_n by the formula

$$\alpha' = \frac{\omega(a, b)\omega(a, a^{n-1})}{\omega_{an}^{2/n}\omega(b, a^{n-1})}, \tag{17}$$

where

$$\omega_{an} = \omega(a, a)\omega(a^2, a)\ldots\omega(a^{n-1}, a).$$

It is easy to see that formula (17) for the factor-system (16) and the relation $(\omega_2)_{c_2 2} = \omega_2(c_2, c_2) = -1$ lead to the value $\alpha' = \frac{\omega_2(c_2, u_2)\omega_2(c_2, c_2)}{(\omega_2)_{c_2 2}\omega_2(u_2, c_2)} = \frac{1\cdot(-1)}{(-1)\cdot(-1)} = -1$, which characterizes namely the projective class K_1 in groups D_n.

Let us calculate the values of function $u_2(r)$ for all r and bring the factor-system (16) to p-equivalent standard form $\omega_2'(r_2, r_1)$, thereby constructing, for the first time, a standard factor-system of the class K_1 – the factor-system $\omega_{(1)}'(r_2, r_1)$ for the group D_2 and all groups isomorphic to it, because, for all point groups with projective representations of the class K_1, of course, the equality $\omega_2'(r_2, r_1) = \omega_{(1)}'(r_2, r_1)$ is satisfied. Here, in the notation of factor-systems, as well as previously, the strokes indicate that these factor-systems are standard, and the lower numerical index in parentheses indicates the class of a factor system.

Let us use some formulas which are general for the groups D_n determining the values of functions $u(r)$ and lead the factor-systems $\omega(r_2, r_1)$ to the standard form. These formulas have a form [1]

$$\begin{aligned}
&u(a^p) = \frac{\omega_{an}^{p/n}}{\omega_{ap}}\varepsilon^p,\\
&u(b^q) = -\frac{\omega^{q/2}(b, b)}{\omega_{am}\omega(a, a)},\\
&u(b^q a^p) = \frac{u(a^p)u(b^q)}{\omega(b^q, a^p)}.
\end{aligned} \tag{18}$$

Since $\alpha' = \varepsilon_2^m = (e^{i2\pi/2})^m = (e^{i\pi})^m = (-1)^m$ and, at the same time, $\alpha' = -1$ for the factor-system (16), m is an odd number for this factor system (for example, one can assume $m = 1$). For an odd m,

$$\varepsilon = i\frac{(\alpha')^{1/2}}{\omega(a, a)}. \tag{19}$$

For the factor-system (16), therefore, $\varepsilon = i\frac{(\alpha')^{1/2}}{\omega_2(c_2, c_2)} = i\frac{(-1)^{1/2}}{-1} = 1$. Taking into account that $(\omega_2)_{c_2 2}^{1/2} = \omega_2^{1/2}(c_2, c_2) = (-1)^{1/2} = i$ and $(\omega_2)_{c_2 1} = 1$, we obtain $u_2(c_2) = \frac{(\omega_2)_{c_2 2}^{1/2}}{(\omega_2)_{c_2 1}}\varepsilon = i$, $u_2(u_2) = -\frac{\omega_2^{1/2}(u_2, u_2)}{\omega_{c_2 1}\omega_2(c_2, c_2)} = -\frac{(-1)^{1/2}}{-1} = i$. Since $u_2' = u_2c_2$ for the ordinary group D_2, we have $u_2(u_2') = \frac{u_2(c_2)u_2(u_2)}{\omega_2(u_2, c_2)} = 1$.

In view of the relation $u_2(e) = 1$ and the fact that the function $u_2(r)$ for the elements e, c_2, u_2 and u_2' of the group D_2 takes the values of 1, i, i and 1, respectively, the factor system (16) is reduced to the p-equivalent standard factor-system $\omega_2'(r_2, r_1)$, using the transformation

$$\omega_2'(r_2, r_1) = \frac{\omega_2(r_2, r_1)u_2(r_2r_1)}{u_2(r_1)u_2(r_2)}. \tag{20}$$

This standard factor-system coincides with the standard factor-system of the class $K_1$of the group D_2

and groups isomorphic to it, i.e., the factor-system $\omega_{(1)}(r_2, r_1)$. It was obtained for the first time and has the form

$\omega'_{(1)}(r_2, r_1)$ — r_1 / r_2	e	c_2	u_2	u'_2
e	1	1	1	1
c_2	1	1	−1	−1
u_2	1	1	1	1
u'_2	1	1	−1	−1

(21)

Using the known [1] characters of the irreducible projective representation $P^{(1)}$ of the class K_1 of the group D_2, the corresponding standard factor-system $\omega'_{(1)}(r_2, r_1)$ and the values of function $u_2(r)$, which are shown in Table 1, *b*), according to formula (4), assuming $\mathbf{k} = \mathbf{k}_\Gamma = 0$, we can easily find the characters of the irreducible spinor representation $\Gamma_5(\mathrm{E}')$ of the group D_2 in the form of characters of its projective representation (Table 1, *b*). The characters of irreducible representations of the double group D'_2 are given in Table 1, *a*) for comparison. It is easy to see that the characters of the spinor representation $\Gamma_5(\mathrm{E}')$ shown in Table 1 *a*) coincide with the calculated characters of the two-valued projective representation $\Gamma_5(\mathrm{E}')$ of the class K_1, which are given in Table 1, *b*).

It should be noted that the characters of the irreducible projective representation $P^{(1)}$ corresponding to a standard factor-system of the class K_1 can be obtained from readily calculated matrices of this representation [1]. Furthermore, from the same matrices, the matrices of the irreducible spinor representation $\Gamma_5(\mathrm{E}')$ can be easily found by formula (3).

It is interesting that, by applying formulas (17–19) to the factor-system (21), we obtain the values of function $u'_2(r)$ for the elements e, c_2, u_2, and u'_2, which are 1, −1, −1, and 1 (for the factor-system (21), as for the factor-system (16), of course, $\alpha' = -1$ and $\varepsilon = -1$), correspondingly, which, as it turns out for transformation (20), leave the factor-system (21) invariant. This means, that the further reduction of the factor-system (21) using formulas (17–19) to the standard form is impossible, and the factor-system (21), indeed, is a standard factor-system of the class K_1 of the group 222 (D_2). The functions $u''_2(r) \equiv u_2(r)$, or $u''_2(r) = u_2(r)u'_2(r)$ themselves become ambiguous, as the complex values of coefficients for the reduction of the factor-system (16) to the standard form $u''_2(r)$ can be taken with the sign "plus" or with the sign "minus" and, for the elements e, c_2, u_2, and u'_2, take the values of 1, i, i and 1 or 1, $-i$, $-i$ and 1, correspondingly. It is also easy to notice that the values of reduction coefficients allowable by formulas (17–19) for the

Table 1. **Characters of: *a* – irreducible representations of the double point group $(222)'(D'_2)$ and *b* – irreducible one-valued vector representations and irreducible two-valued projective representations of the point group $(222)(D_2)$. Upper part of table 1, *b* shows the characters of irreducible projective representation of the K_1 class of the $(222)(D_2)$ group, which correspond to the standard factor-system of the class K_1 of the group $(222)(D_2)$ – factor system $\omega'_{(1)}(r_2, r_1)$ of the group 222 (D_2) and the values of function $u_2(r)$, corresponding to the factor-system $\omega_2(r_2, r_1)$ of the class K_1 of this group reduce it to the *p*-equivalent standard factor-system $\omega'_2(r_2, r_1)$ of the group 222 (D_2), which, in this case, coincides with the factor-system $\omega'_{(1)}(r_2, r_1)$**

a)

$(222)'$ (D'_2)	e	q	c_2, qc_2	u_2, qu_2	u'_2, qu'_2
Γ_1 A_1	1	1	1	1	1
Γ_2 A_2	1	1	1	−1	−1
Γ_3 B_1	1	1	−1	1	−1
Γ_4 B_2	1	1	−1	−1	1
Γ_5 E'	2	−2	0	0	0

b)

222 (D_2)	e	c_2	u_2	u'_2
$\mathrm{P}^{(1)}$	2	0	0	0

222 (D_2)	e	c_2	u_2	u'_2
$u_2(r)$	1	i	i	1

222 (D_2)	e	c_2	u_2	u'_2
Γ_1 A_1	1	1	1	1
Γ_2 A_2	1	1	−1	−1
Γ_3 B_1	1	−1	1	−1
Γ_4 B_2	1	−1	−1	1
Γ_5 E'	2	0	0	0

elements of the group D_2, listed in the above order, form two additional sets 1, $-i$, i, -1 and 1, i, $-i$, -1. This also leads the factor system (16) to the standard form (21). Without loss of generality, it is sufficient to use only one of the above cases, and we will use, as was done in Table 1, *b*), only the complex values of the reduction coefficients with the "plus" sign for the elements e, c_2, u_2, and u_2', i.e., the values of 1, i, i and 1, respectively.

Let us consider the group D_3 containing 6 elements: e, c_3, c_3^2, $(u_2)_1$, $(u_2)_2$, and $(u_2)_3$. The constituting elements in this group are $a = c_3(c_{3z})$ and $b = (u_2)_1(c_{2x})$. The obvious defining relations $a^6 = e$ ($a^3 = q$) and $b^4 = e$ ($b^2 = q$) for the constituting element are fulfilled in the double group D_3'.

Let us find a commuting defining relation for the constituting elements of the double group D_3'. For the ordinary group D_3, this relation has the form $ab = ba^2$.

Considering c_3 as $c_\ell(2\pi/3)$ ($\ell \parallel Oz$), assuming $f = q(u_2)_1 = qc_{\ell'}(\pi)$ ($\ell' \parallel Ox$), and taking into account that $f^{-1} = (u_2)_1 = c_{\ell'}(\pi)$ and $f^{-1}\ell = c_{\ell'}(\pi)\ell = -\ell$, relation (12) for the double groups yields $c_{\ell'}(\pi)c_\ell(2\pi/3)qc_{\ell'}(\pi) = c_{-\ell}(2\pi/3)$. Since $c_{-\ell}(2\pi/3) = qc_\ell(4\pi/3) = qc_\ell^2(2\pi/3)$, we find $q(u_2)_1c_3(u_2)_1 = qc_3^2$.

Multiplying this equation on the left by $(u_2)_1$, we obtain

$$c_3(u_2)_1 = q(u_2)_1c_3^2 \quad \text{or} \quad ab = qba^2, \tag{22}$$

which is a commuting defining relation for the constituting elements of the double group D_3'. It is significant that the operation q is also included into the commuting defining relation for constituting elements of the double group D_3', as well as into the commuting defining relation for constituting elements of the double group D_2' (14).

In order to determine the elements $(u_2)_2$ and $(u_2)_3$ in the double group D_3', in view of the definition of the above-considered element u_2' in the double group D_2', Eq. (12) also can be used.

Indeed, the relations $c_3(u_2)_1qc_3^2 = (u_2)_2$ and $c_3^2(u_2)_1qc_3 = (u_2)_3$ obtained on the basis of this equality can be considered as the definition of elements $(u_2)_2$ and $(u_2)_3$ in the double group D_3'. Using relation (22), it is easy to obtain, from these relations, that

$$\begin{aligned} &(u_2)_2 = q(u_2)_1c_3 \quad \text{or} \quad (u_2)_2 = qba, \\ &(u_2)_3 = (u_2)_1c_3^2 \quad \text{or} \quad (u_2)_3 = ba^2. \end{aligned} \tag{23}$$

Having the defining relations for the constituting elements and relations (22) and (23), it is not difficult to find the factor-system $\omega_2(r_2, r_1)$ for the group D_3. This factor-system has the form

$\omega_2(r_2, r_1)$ / r_2	r_1	e	c_3	c_3^2	$(u_2)_1$	$(u_2)_2$	$(u_2)_3$
b^0a^0	e	1	1	1	1	1	1
b^0a^1	c_3	1	1	−1	−1	−1	−1
b^0a^2	c_3^2	1	−1	−1	1	1	1
b^1a^0	$(u_2)_1$	1	−1	1	−1	1	−1
qb^1a^1	$(u_2)_2$	1	−1	1	−1	−1	1
b^1a^2	$(u_2)_3$	1	−1	1	1	−1	−1

(24)

All factor-systems belonging to the class K_0 and all irreducible projective representations belonging to the group D_3 (group D_n with an odd n) are p-equivalent to the ordinary vectorial groups. As was already mentioned, the factor-systems with all the elements equal to 1 are standard factor-systems of the class K_0 in all groups. It is easy to see that the factor-system (24) is reduced to the p-equivalent standard factor-system $\omega_2'(r_2, r_1)$ coinciding, in this case, with the standard factor-system of the class K_0 of the group D_3, i.e. the factor-system $\omega_{(0)}'(r_2, r_1)$ of the group D_3, all elements of which are equal to 1, using transformation (20), where the function $u_2(r)$ for the elements e, c_3, c_3^2, $(u_2)_1$, $(u_2)_2$, and $(u_2)_3$ has the values of 1, -1, 1, i, i and i, correspondingly [1],

$$\begin{aligned} &u_2(c_3^p) = e^{ip\pi}(p = 0, 1, 2), \\ &u_2[(u_2)_\ell^q] = \varepsilon_4^q = \left(e^{i2\pi/4}\right)^q = \\ &= e^{iq\pi/2}(\ell = 1, 2, 3;\ q = 0, 1). \end{aligned} \tag{25}$$

The equality $\omega_2'(r_2, r_1) = \omega_{(0)}'(r_2, r_1)$, which is fulfilled in this case, is a criterion of correctness of the above-determined values of the function $u_2(r)$.

In accordance with formula (4), let us multiply the characters (Table 2, *b*) of irreducible ordinary vector representations of the group D_3 by the values of function $u_2(r)$ given in the top part of Table 2, *b*. We get the characters of irreducible spinor representations (Table 2, *b*) of the group D_3 in the form of the characters of their projective representations. The characters of irreducible representations of the double group D'_3 are given in Table 2, a for comparison. It is easy to see that the characters of spinor representations given in Table 2, a coincide with the calculated characters of two-valued projective representations of the class K_0, given in Table 2, b.

In the same manner, we can obtain the factor-systems $\omega'_2(r_2, r_1)$ and $\omega'_{(1)}(r_2, r_1)$, and the values of coefficients $u_2(r)$ and to construct irreducible spinor representations also in groups containing the axes of higher orders.

Table 2. **Characters of: a – the irreducible representations of the double point group $(32)'(D'_3)$ and b – irreducible one-valued vector representations and the irreducible two-valued projective representations of the point group $32(D_3)$. Both parts of the table shows the way of association of the representations (complex conjugate, in this case) with regard for the time-reversal invariance of states. Upper part of Table 2, b shows the values of function $u_2(r)$, which convert the factor-system $\omega_2(r_2, r_1)$ of the group $32(D_3)$, which belongs to the class K_0, to the p-equivalent standard factor-system $\omega'_2(r_2, r_1)$ of this group, which coincides, in this case, with the standard factor-system of the class K_0 of the group $32(D_3)$ – factor-system $\omega'_{(0)}(r_2, r_1)$ of the group $32(D_3)$, all coefficients of which are equal to 1**

a)

$(32)'$	(D'_3)	e	q	$c_3,\ qc_3^2$	$c_3^2,\ qc_3$	$3u_2$	$3qu_2$
Γ_1	A_1	1	1	1	1	1	1
Γ_2	A_2	1	1	1	1	-1	-1
Γ_3	E	2	2	-1	-1	0	0
$\Gamma_4+\Gamma_5 <\ \Gamma_4$	$E'_1+E'_2 <\ E'_1$	1	-1	-1	1	i	$-i$
Γ_5	E'_2	1	-1	-1	1	$-i$	i
Γ_6	E'_3	2	-2	1	-1	0	0

b)

32	(D_3)	e	c_3	c_3^2	$3u_2$
	$u_2(r)$	1	-1	1	i

32	(D_3)	e	c_3	c_3^2	$3u_2$
Γ_1	A_1	1	1	1	1
Γ_2	A_2	1	1	1	-1
Γ_3	E	2	-1	-1	0
$\Gamma_4+\Gamma_5 <\ \Gamma_4$	$E'_1+E'_2 <\ E'_1$	1	-1	1	i
Γ_5	E'_2	1	-1	1	$-i$
Γ_6	E'_3	2	1	-1	0

Thus, we have presented the method of construction of the factor-systems $\omega_2(r_2, r_1)$ and the irreducible spinor representations of the point groups in the form of their projective representations, which allows solving the problem of finding the irreducible two-valued representations of wave vector groups and full space groups. The groups 222 (D_2) and 32 (D_3), which were chosen as illustrations of the applicability of the proposed method of construction of the factor systems $\omega_2(r_2, r_1)$ and the irreducible spinor representations, are the simplest examples of non-Abelian groups, whose factor-systems $\omega_2(r_2, r_1)$ exhausting all possible situations belong either to the class K_1, as in case of the group D_2, or to the class K_0, as in case of the group D_3. It is also significant that the method allowed one to find, for the first time, the factor-system $\omega'_{(1)}(r_2, r_1)$, which is a standard factor-system of the class K_1 for the group D_2 having irreducible projective representations, which belong to the class K_1, and for all groups isomorphic to it, and to find the values of function $u_2(r)$ for the group D_3, bringing the factor-system $\omega_2(r_2, r_1)$ constructed for it to the p-equivalent standard factor-system of the class K_0, all the coefficients of which are equal to 1.

In conclusion, we note that the essence of Bethe's method, in our opinion, is the introduction of the operation q, which correctly reflects the transformation properties of spinors. This method seems more logical and can be more precisely mathematically used in constructing the factor-systems $\omega_2(r_2, r_1)$ and the two-valued representations of the point and space symmetry groups in the form of projective representations of the ordinary point group, by preserving their systematics and hierarchy, and not in the form of true irreducible representations of abstract double groups, since assigning the sequence numbers for which, as a rule, is arbitrary.

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РОЗВИТОК МЕТОДУ
БЕТЕ ДЛЯ ПОБУДОВИ ДВОЗНАЧНИХ
ПРЕДСТАВЛЕНЬ ПРОСТОРОВИХ
ТА ДВОЗНАЧНИХ ПРОЕКТИВНИХ
ПРЕДСТАВЛЕНЬ ТОЧКОВИХ ГРУП

Р е з ю м е

Розглянуто методику побудови двозначних представлень просторових та двозначних проективних представлень точкових груп. Представлено метод побудови фактор-систем $\omega_2(r_2, r_1)$, які відображають перетворення хвильових функцій квантових систем з напівцілим спіном, і які є необхідними для знаходження двозначних незвідних проективних представлень точкових груп. Цей метод ґрунтується на введенні в ролі додаткового елемента симетрії операції q, вперше використаної Бете. На прикладі груп 222 (D_2) та 32 (D_3) показано, яким чином вводяться співвідношення, що дозволяють зробити однозначними алгебру подвійних груп та, зокрема, їх таблиці множення. Показано, яким чином на основі співвідношень, що обговорюються, будується вперше представлена для групи 222 стандартна фактор-система класу K_1 – фактор-система $\omega'_{(1)}(r_2, r_1)$. Обговорюються також в цілому роль та можливості методу Бете та його модифікацій в побудові двозначних представлень точкових та просторових груп.