FACTORIZATION OF THE GROUP O_4 AND THE HYDROGEN ATOM

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The relation between $SU_2 \otimes SU_2$ and O_4 is studied with a method different from the usual way, leading to the well-known results of classical quantum mechanics for the hydrogen atom.

The quantum mechanical role of continuous groups is scarcely to be overestimated since WIGNER's classical work [1]. He obtained his first success by the interpretation of the angular momentum, connecting this physical quantity with the rotation group. Later on other continuous groups became of great importance, too. May it suffice to point to the group SU_3, very important in the theory of elementar particles. Investigation into the symmetry of the hydrogen atom began early. FOCK [2], then BARGMANN [3] pointed out that the hydrogen atom has a symmetry higher than O_3, namely, O_4 symmetry. In this connection GYÖRGYI [4] obtained important results. All this points to the circumstance that the group O_4 deserves further attention from the point of view of physical applications. GYÖRGYI's mentioned results can be not only formulated in an other way [5] but also developed with respect to applications. A good review of the problem is given by MICHEL [6].

The semi-simple Lie-groups [7] can be classified according to the classification of the correnponding Lie-algebras. Accordingly, the group O_n is not simple in the case of even n, *i.e.* its algebra has a commutative ideal; this means that, for *e.g* $n=4$, O_4 can be factorized. In this paper we study this factorization and, on this basis, give the irreducible representation of the group. This conception seems also to be more convenient from the point of view of applications.

Factorization of the group O_4

Let us start from the group SU_2. This consists of all unitary matrices of determinant $+1$ of the two-dimensional complex vector space. The group SU_2 is closely connected with the rotation group of the real three-dimensional space. More precisely, there are two matrices differing in sign which correspond to a rotation of the first kind in SU_2; this circumstance will be, however, neglected in the following as irrelevant.

The irreducible representations of SU_2 can be obtained in the well-known way [1]. The irreducible representations can be distinguished by a number j ($j=0$, $1/2$, $1, \ldots$).

Let us denote be D_j the corresponding representation, which is of dimension $2j+1$. The defining representation belongs to $j=1/2$. The connection with the rotation group can be built up through the representation D_1.

The rotation group O_3 of the three-dimensional space can be parametrized is several equivalent ways: besides the Eulerian angles, the rotations can be characterized also by a vector the length of which is determined by the angle of rotation $\varphi (0 \leqq \varphi < \pi)$ and its direction by the polar angles of $\Phi (0 \leqq \Phi < 2\pi)$ and $\Theta (0 \leqq \Theta < \pi)$.

Starting from given groups, a further group can be defined by direct product. The direct product $G = G_1 \otimes G_2$ of two groups G_1 and G_2 is a set the elements of which consist of all pairs (g_1, g_2), where $g_1 \in G_1$, $g_2 \in G_2$. Among the elements of the resulting set, multiplication can be defined by

$$(g_1, g_2)(g_1', g_2') = (g_1 g_1', g_2 g_2'). \tag{1}$$

For this multiplication G is a group. Let us recall the pertinent algebraic theorems: (i) the representations of a direct product are given by the direct product of the representations of the factor groups; (ii) the trace of the direct product of two matrices is the product of the two traces; (iii) the representation of a direct product built up from irreducible factors is irreducible.

Accordingly, the direct product $SU_2 \otimes SU_2$ is a group with six parameters. Let us denote the parameters by Φ, Θ, φ and Φ', Θ', φ', respectively. The defining representation of the direct product is obtained by the direct product of the defining representations. Let A be a matrix of the defining representation SU_2

$$A = \begin{pmatrix} \alpha & \beta \\ -\beta^* & \alpha^* \end{pmatrix}, \quad \alpha\alpha^* + \beta\beta^* = 1, \tag{2}$$

where α and β are otherwise arbitrary complex numbers. Another element (with primed parameters) is

$$B = \begin{pmatrix} a & b \\ -b^* & a^* \end{pmatrix}, \quad aa^* + bb^* = 1. \tag{3}$$

The set of all matrices

$$T = A \otimes B = (t_{ij}) = \begin{pmatrix} \alpha a & \alpha b & \beta a & \beta b \\ -\alpha b^* & \alpha a^* & -\beta b^* & \beta \alpha^* \\ -\beta^* \alpha & -\beta^* b & \alpha^* a & \alpha^* b \\ \beta^* b^* & -\beta^* a^* & -\alpha^* b^* & \alpha^* a^* \end{pmatrix} \tag{4}$$

gives the defining representation of $SU_2 \otimes SU_2$.

The matrices T can be considered as transformations of the complex vector space spanned by the basis vectors e_1, e_2, e_3, e_4. The elements of this space are linear expressions of the following form

$$v = c_1 e_1 + c_2 e_2 + c_3 e_3 + c_4 e_4. \tag{5}$$

By T, the components c_i of vector v transform according to

$$c_i' = \sum_{j=1}^{4} t_{ij} c_j \equiv t_{ij} c_j, \quad (i = 1, 2, 3, 4). \tag{6}$$

Making use of the properties of SU_2, we obtain

$$c_1' c_4' - c_2' c_3' = c_1 c_4 - c_2 c_3, \tag{7}$$

i.e. an invariant expression. Introducing the quantities

$$x_1 = \frac{c_1+c_4}{2}, \; x_2 = -i\frac{c_1-c_4}{2}, \; x_3 = \frac{c_2-c_3}{2}, \; x_4 = -i\frac{c_2+c_3}{2} \tag{8}$$

for which

$$x_i x_i = c_1 c_4 - c_2 c_3, \tag{9}$$

thus $x_i x_i$ will also be invariant.

The transformations of the x_i-s can be obtained from Eq. (8) (see Appendix I). By these transformations real x_i-s are converted into real ones. Therefore the quantities $x=(x_1, x_2, x_3, x_4)$ can be considered as vectors of a real four-dimensional space, and the T-s as their transformations. According to Eqs. (7) and (9), these transformations leave the length of the vector invariant.

The elements of the group O_4 consist of all real 4×4 matrices which leave the $x_i x_i$ invariant. Accordingly, all elements of $SU_2 \otimes SU_2$ belong to O_4: $SU_2 \otimes \otimes SU_2 \subseteqq O_4$. If all elements of O_4 have a corresponding element in $SU_2 \otimes SU_2$, then the relation will become an isomorphism. As a proof, let us calculate the infinitesimal elements of both groups and the infinitesimal operators of the commutation relations (Appendix II). The commutation relations and structure constants of both groups are identical. Thus both groups are isomorphic at least for infinitesimal quantities.

Representations and their decompositions

The above connections between $SU_2 \otimes SU_2$ and O_4 being valid, the representations of the former will be representations of the latter as well. An irreducible representation of $SU_2 \otimes SU_2$, being derived from two irreducible representations of SU_2, can be characterized by two numbers $(j; j')$. The dimensions of the representation $(2j+1)(2j'+1)$ can be found for some cases in Table I. Especially, the dimensions of the irreducible representations pertaining to $j'=j$ are the squares of the natural numbers. The irreducible representations of O_4 are given by the matrices $D_j \otimes D_{j'}$.

The question of decomposing according to O_3 the representations $D_j \otimes D_{j'}$ of O_4, which in general are clearly reducible representations of O_3, seems to be of importance with respect to applications.

This problem can be solved on the analogy of the procedure used for finite groups. Instead of summing for all elements of the group, which plays an important role for finite groups, integration is to be used in the case of continuous groups [8].

Table I

j' \ j	0	1/2	1	3/2	2
0	1	2	3	4	5
1/2	2	4	6	8	10
1	3	6	9	12	15
3/2	4	8	12	16	20
2	5	10	15	20	25

Let the number $f(g)$ conrespond to an element $g \in G$, then the conresponding integral will be

$$\frac{1}{V} \int_G f(g)\, dV(g), \tag{10}$$

where V is the volume of the parameter space, and $dV(g)$ the volume element around g. In the case of group O_3, the latter can be written [1] as

$$dV(g) = g(E) 2(1-\cos \Phi) \sin \varphi \, d\Phi \, d\Theta \, d\varphi \tag{11}$$

where $g(E)$ is the so called weight function. Especially, with $g(E)=1$ we obtain

$$V = 8\pi^2. \tag{12}$$

The expressions $f(g)$, important for the problem, are mostly matrix elements and traces of the representations. For these the following theorems are valid. The traces of the irreducible representations j and j' fulfil the orthogonality relation [8]

$$\frac{1}{V} \int_G \chi_j(g) \chi_{j'}^*(g)\, dV(g) = \delta_{jj'}. \tag{13}$$

A reducible representation D can be decomposed into the direct sum of irreducible representations in the form

$$D = n_1 D_{j_1} \oplus \ldots \oplus n_k D_{j_k} \tag{14}$$

where n_i is the multiplicity of the irreducible representation i. If the trace of the representation D is $\chi(g)$, then

$$n_i = \frac{1}{V} \int_G \chi(g) \chi_{j_i}^*(g)\, dV(g). \tag{15}$$

Let D be an irreducible representation of O_4, and D_{j_i} one of O_3, then Eq. (15) gives the number of the corresponding irreducible components. By these the decomposition in Eq. (14) is determined; some of the decompositions are presented in Table II.

Table II

Decompositions of $D_{j'} \otimes D_j$

$D_{j'}$ \ D_j	D_0	$D_{1/2}$	D_1	$D_{3/2}$	D_2
D_0	D_0	$D_{1/2}$	D_1	$D_{3/2}$	D_2
$D_{1/2}$	$D_{1/2}$	$D_0 \oplus D_1$	$D_{1/2} \oplus D_{3/2}$	$D_1 \oplus D_2$	$D_{3/2} \oplus D_{5/2}$
D_1	D_1	$D_{1/2} \oplus D_{3/2}$	$D_0 \oplus D_1 \oplus D_2$	$D_{1/2} \oplus D_{3/2} \oplus D_{5/2}$	$D_1 \oplus D_2 \oplus D_3$
$D_{3/2}$	$D_{3/2}$	$D_1 \oplus D_2$	$D_{1/2} \oplus D_{3/2} \oplus D_{5/2}$	$D_0 \oplus D_1 \oplus D_2 \oplus D_3$	$D_{1/2} \oplus D_{3/2} \oplus D_{5/2} \oplus$ $\oplus D_{7/2}$
D_2	D_2	$D_{3/2} \oplus D_{5/2}$	$D_1 \oplus D_2 \oplus D_3$	$D_{1/2} \oplus D_{3/2} \oplus D_{5/2} \oplus$ $\oplus D_{7/2}$	$D_0 \oplus D_1 \oplus D_2 \oplus$ $\oplus D_3 \oplus D_4$

Group O_4 and the hydrogen atom

The hydrogen atom is of O_4 symmetry, therefore its eigenfunctions transform according to the irreducible representations of O_4, and its eigenvalues can be arranged according to the latter. The irreducible representations of O_4 can be characterized by the numbers (j, j'), but not all combinations have a real physical meaning; only the case $j'=j$ is realized. Except for the case $j'=j=0$, the irreducible representations are not unidimensional (Table I); the corresponding states are degenerate. What are the differences between the corresponding states?

From the infinitesimal operators belonging to group O_4 the combination

$$C = A_1^2+A_2^2+A_3^2+B_1^2+B_2^2+B_3^2 \tag{16}$$

(CASIMIR operator) can be formed. This is commutable with every A_i and B_i. The operator C is connected with the energy of the hydrogen atom [5]. This operator is commutable with $B^2 = B_1^2+B_2^2+B_3^2$, which is in similar connection with O_3, as C with O_4. The relations

$$[C, B^2] = 0, \quad [B^2, B_3] = 0, \quad [C, B_3] = 0 \tag{17}$$

will hold. There exist no further combinations of the infinitesimal operations which, joint to the operators C, B^2, B_3, would give a mutually commutable set. Thus there exist only three such operators. B^2 is connected with the absolute value of the angular momentum, and B_3 (respectively iB_3) with the third component of the latter. These results are well known from classical quantum mechanics.

Appendix I

From Eq. (6), using Eq. (4), detailed expressions for the c_i'-s can be obtained. Substituting these in Eq. (8) and rearranging, the x_i'-s can be found:

$$\begin{aligned}
x_1' &= x_1\frac{\alpha a-\beta^*b^*+\alpha^*a^*-\beta b}{2}+x_2 i\frac{\alpha a-\beta^*b^*+b\beta-\alpha^*a^*}{2}+\\
&\quad +x_3\frac{-\beta^*a^*-\alpha b-\alpha^*b^*-\beta a}{2}+x_4 i\frac{\alpha^*b^*-\alpha b-\beta^*a^*+\beta a}{2},\\
x_2' &= x_1 i\frac{-\beta^*b^*-\alpha a+\beta b+\alpha^*a^*}{2}+x_2\frac{\beta^*b^*+\alpha a+\beta b+\alpha^*a^*}{2}+\\
&\quad +x_3 i\frac{\alpha b-\beta^*a^*+\beta a-\alpha^*b^*}{2}+x_4\frac{\beta a-\alpha^*b^*-\alpha b+\beta^*a^*}{2},\\
x_3' &= x_1\frac{b^*\alpha+\beta^*a+\alpha^*b+\beta a^*}{2}+x_2 i\frac{\alpha b^*+\beta^*a-\alpha^*b-\beta a^*}{2}+\\
&\quad +x_3\frac{\alpha a^*-\beta^*b+\alpha^*a-\beta b^*}{2}+x_4 i\frac{\alpha a^*-\beta^*b+\beta b^*-\alpha^*a}{2},\\
x_4' &= x_1 i\frac{\beta^*a-\alpha b^*+\alpha^*b-\beta a^*}{2}+x_2\frac{\alpha b^*-\beta^*a+\alpha^*b-\beta a^*}{2}+\\
&\quad +x_3 i\frac{-\alpha a^*-\beta^*b+\beta b^*+\alpha^*a}{2}+x_4\frac{\alpha a^*+\beta^*b+\beta b^*+\alpha^*a}{2}.
\end{aligned} \tag{18}$$

Appendix II

The elements of the defining representation of SU_2 can be also expressed by φ, Φ, Θ

$$\alpha = \cos\frac{\varphi}{2} - i\sin\frac{\varphi}{2}\cos\Phi, \quad \beta = -e^{i\Theta}\sin\frac{\varphi}{2}\sin\Phi. \tag{19}$$

An element will be infinitesimal if the angle of rotation φ is infinitesimal for Φ and Θ. In the case of small φ, Eq.-s (19) can be written in the form

$$\delta\alpha = 1 - i\frac{\varphi}{2}\cos\Phi, \quad \delta\beta = -\frac{\varphi}{2}\sin\Phi e^{i\Theta} \tag{20}$$

and, for the other factor as

$$\delta a = 1 - i\frac{\varphi'}{2}\cos\Phi', \quad \delta b = -\frac{\varphi'}{2}\sin\Phi' e^{i\Theta}. \tag{21}$$

Substituting these into Eq. (18) and neglecting the terms of second and higher order, we obtain

$$\delta T' = \begin{pmatrix} 1 & a_3 & -a_1 & a_2 \\ -a_3 & 1 & b_2 & b_1 \\ a_1 & -b_2 & 1 & b_3 \\ -a_2 & -b_1 & -b_3 & 1 \end{pmatrix} \tag{22}$$

where the notations

$$\begin{aligned} a_1 &= -\frac{\varphi}{2}\sin\Phi\cos\Theta - \frac{\varphi'}{2}\sin\Phi'\cos\Theta', \\ a_2 &= \frac{\varphi}{2}\sin\Phi\sin\Theta - \frac{\varphi'}{2}\sin\Phi'\sin\Theta', \\ a_3 &= \frac{\varphi}{2}\cos\Phi + \frac{\varphi'}{2}\cos\Phi' \end{aligned} \tag{23}$$

and

$$\begin{aligned} b_1 &= -\frac{\varphi}{2}\sin\Phi\cos\Theta + \frac{\varphi'}{2}\sin\Phi'\cos\Theta', \\ b_2 &= \frac{\varphi}{2}\sin\Phi\sin\Theta + \frac{\varphi'}{2}\sin\Phi'\sin\Theta', \\ b_3 &= \frac{\varphi}{2}\cos\Phi - \frac{\varphi'}{2}\cos\Phi' \end{aligned} \tag{24}$$

are used. The corresponding infinitesimal operators can be calculated from

$$\left(\frac{\partial\delta T'}{\partial a_i}\right)_{a_i=0,\, b_i=0} = A_i, \quad \left(\frac{\partial\delta T'}{\partial b_i}\right)_{a_i=0,\, b_i=0} = B_i. \tag{25}$$

Then, the commutation relations will be

$$\begin{aligned} A_iA_j - A_jA_i &= B_k \\ A_iB_j - B_jA_i &= A_k \\ B_iA_j - A_jB_i &= A_k \\ B_iB_j - B_jB_i &= B_k \end{aligned} \qquad (ijk = 123, 231, 312) \tag{26}$$

and

$$A_iB_i - B_iA_i = 0 \qquad (i = 1, 2, 3). \tag{27}$$

Let a matrix g of O_4 be

$$g = \begin{pmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{pmatrix} \tag{28}$$

for which

$$a_{ni}a_{nk} = \delta_{ik} \qquad (i, k = 1, 2, 3, 4); \tag{29}$$

this means 10 relations for 16 real a_{ik}. Let us write these in the form

$$a_{ik} = \delta_{ik} + c_{ik} \tag{30}$$

and let the c_{ik} be infinitesimal. Then

$$c_{ki} = -c_{ik}, \quad c_{ii} = 0, \tag{31}$$

therefore the infinitesimal form of Eq. (28), using the notation

$$\begin{aligned} c_{12} &= \varepsilon_3, \quad c_{13} = -\varepsilon_1, \quad c_{14} = \varepsilon_2, \\ c_{23} &= \delta_2, \quad c_{24} = \quad \delta_1, \quad c_{34} = \delta_3 \end{aligned} \tag{32}$$

will be

$$g = \begin{pmatrix} 1 & \varepsilon_3 & -\varepsilon_1 & \varepsilon_2 \\ -\varepsilon_3 & 1 & \delta_2 & \delta_1 \\ \varepsilon_1 & -\delta_2 & 1 & \delta_3 \\ -\varepsilon_2 & -\delta_1 & \delta_3 & 1 \end{pmatrix}. \tag{33}$$

The infinitesimal operators will be given by

$$\left(\frac{\partial g}{\partial \varepsilon_i}\right)_{\varepsilon_i=0,\, \delta_i=0} = A_i', \quad \left(\frac{\partial g}{\partial \delta_i}\right)_{\varepsilon_i=0,\, \delta_i=0} = B_i'. \tag{34}$$

For these the same commutation relations will hold as for A_i-s and B_i-s.

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РАЗЛОЖЕНИЕ ГРУППЫ O_4 И АТОМ ВОДОРОДА

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Изучена связь между группами $SU_2 \otimes SU_2$ и O_4 новым методом, отличающимся от известного, и получены результаты классической квантовой механики для атома водорода.