O_4 REPRESENTATIONS AND THE SPECTRA OF HYDROGEN AND HELIUM

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The correspondence between some of the representations of the O_4 group and the hydrogen levels is stated again. The speciality of the occurring representations is pointed out. The helium states are obtained using $O_4 \otimes O_4 \otimes S_2$.

The group theoretical classification of hadrons based on the assumption that mesons and baryons form SU_3 multiplets has proved very fruitful. But only some of the irreducible representations of SU_3 appear really as physical states. Supposing that quarks exist, the speciality of these representations would be clear. But, as there have not been found any quarks yet, it is still a puzzle why these and not other representations do actually occur in nature. So it may be interesting to study the speciality of the occurring representations in the case of other well-known problems.

As it was shown by FOCK [1, 2], the Schrödinger equation of the hydrogen atom can be transformed into an integral equation in the space of the square integrable functions $\Psi(\vec{\xi})$ ($\vec{\xi} \in S^3$) on the four-dimensional unit sphere S^3. The Hamiltonian $\mathbf{H}(\vec{\xi})$ becomes an integral operator with a kernel invariant under rotations in the four-dimensional space. These rotations form a group, the group O_4. Let $g \in O_4$, then $\mathbf{H}(g\vec{\xi}) = \mathbf{H}(\vec{\xi})$. More generally, for each $g \in O_4$ let $\Psi(g^{-1}\vec{\xi}) = \mathbf{T}(g)\Psi(\vec{\xi})$, where $\mathbf{T}(g)$ is an operator in the space of the Ψ-s. This defines a mapping $g \to \mathbf{T}(g)$ *i.e.* a representation of the group, called quasiregular representation. It can be seen that $\mathbf{T}(g)$ commutes with $\mathbf{H}$ for each $g \in O_4$:

$$\mathbf{T}(g)\mathbf{H}(\vec{\xi})\Psi(\vec{\xi}) = \mathbf{H}(g^{-1}\vec{\xi})\Psi(g^{-1}\vec{\xi}) = \mathbf{H}(\vec{\xi})\mathbf{T}(g)\Psi(\vec{\xi}).$$

To find the possible energy levels, we have to decompose our representation $\mathbf{T}(g)$ into a direct sum of irreducible components.

The four-dimensional homogeneous harmonic polynomials of degree k ($k=0, 1, \ldots$) form a complete set on the four-dimensional unit sphere. They are of the form

$$h_4^k(\vec{x}) = \sum_{\alpha_1+\alpha_2+\alpha_3+\alpha_4=k} c_{\alpha_1\alpha_2\alpha_3\alpha_4} x_1^{\alpha_1} x_2^{\alpha_2} x_3^{\alpha_3} x_4^{\alpha_4}$$

and

$$\sum_{i=1}^{4} \frac{\partial^2}{\partial x_i^2} h_4^k(\vec{x}) = 0.$$

The value of $h_4^k(\vec{x})$ in any point is uniquely determined by its value on the unit sphere point $\frac{\vec{x}}{|\vec{x}|}$. The functions $h_4^k(\vec{\xi})$ are the four-dimensional spherical harmonics; there exist $(k+1)^2$ linearly independent such functions for each k.

These functions span a space H_4^k of dimension $(k+1)^2$ which can be shown to be invariant and irreducible under $\mathbf{T}(g)$. This means that we have decomposed our representation $\mathbf{T}(g)$ into the irreducibles $\mathbf{T}_4^k(g)$-s which act in the subspaces H_4^k. The subspaces H_4^k are usually characterized by $k+1=n$. The dimensionality of H_4^k is then n^2, which means that each level is n^2-fold degenerate. The spherical harmonics are the eigenfunctions.

Now let us take the three-dimensional rotation group O_3, which is clearly a subset of O_4. Reducing $\mathbf{T}_4^k(g)$ into the direct sum of the irreducible representations of O_4, we find that

$$\mathbf{T}_4^k(g) = \sum_{l=0}^{k} \mathbf{T}_3^l(g), \quad g \in O_3,$$

where the $\mathbf{T}_3^l(g)$-s are the $2l+1$ dimensional representations of O_3. We see that $l=0, 1, \ldots, n-1$.

Now the fact which we want to point out is that the representations $\mathbf{T}_4^k(g)$, though infinitely many of them exist, do not exhaust all the possible irreducible representations. A general irreducible representation of O_4 is labelled by two indices [3]. Thus our representations are very special, as they are labelled only by one integer k. The characteristic feature of the $\mathbf{T}_4^k(g)$-s is that they are subrepresentations of the quasiregular representation.

In the space where $\mathbf{T}_4^k$ acts there is always a vector, namely x_4^k, which is left invariant by all $\mathbf{T}_4^k(h)$ for each $h \in O_3$, because it acts only on x_1, x_2 and x_3.

The interesting fact is that the $\mathbf{T}_4^k(g)$-s are the only irreducible representations of O_4 which have this property, *i.e.* restricting them to O_3, there exists a vector in their space, invariant under all operators of the representation [4]. In the language of physics this means that, among the representations of O_4, only the $\mathbf{T}_4^k(g)$-s possess in their representation space spherically symmetric states in the three-dimensional sense, *i.e.* s states.

The above correspondence between some of the representations of O_4 and the energy levels of hydrogen gives the possibility to make a pure group-theoretical classification of the energy levels of helium. The approximate symmetry group is here the direct product group $O_4 \otimes O_4 \otimes S_2$. S_2 is the two-element permutation group and appears because the system is invariant under the operation of interchanging the two electrons. The Coulomb interaction between the two electrons breaks the $O_4 \otimes O_4 \otimes S_2$ symmetry and the real symmetry of this system is only the $O_3 \otimes S_2$ group.

The appropriate irreducible representations of $O_4 \otimes O_4 \otimes S_2$ are the direct product representations $\mathbf{T}_4^{k_1} \otimes \mathbf{T}_4^{k_2} \otimes \mathbf{T}_s^i \equiv \mathbf{T}^{k_1 k_2 i}$ where the $\mathbf{T}_4^{k_i}$-s are the representations of O_4, and $\mathbf{T}_s^i$ is one of the two possible irreducible representations of S_2, namely $\mathbf{T}_s^+$ or $\mathbf{T}_s^-$. Their invariant subspaces are the symmetric and antisymmetric two-electron functions, respectively.

In the case when $k_1>0$, $k_2>0$, the energy levels of the doubly excited atoms fall into the continuous spectrum of the singly ionized helium atom and so they are optically unobservable. Thus we shall consider only the case $k_2=0$.

Now if we restrict the $T^{k_1 0i}$ representations of $O_4 \otimes O_4 \otimes S_2$ to $O_3 \otimes S_2$, they will become reducible. After finding the irreducible components we obtain some levels, but they do not give the true multiplicities.

We must take into account the spin of the electrons, too. The one-electron spin states belong to the self-representation of SU_2 [5]. This is a double valued representation of O_3 and we write it $T_3^{1/2}$. The two-electron spin states belong to the irreducible parts of $T_3^{1/2} \otimes T_3^{1/2}$. These are the T_3^0 and T_3^1 representations of O_3. The functions that span the space of T_3^1 are symmetric, while those of T_3^0 are antisymmetric when interchanging the two electrons. T_3^0 and T_3^1 are one- and three-dimensional and the corresponding states are the singlet and triplet states, respectively. The helium states belong to those representations of $O_3 \otimes S_2$ which are irreducible parts of $T^{k0+} \otimes T_3^0$ and $T^{k0-} \otimes T_3^1$. According to the Pauli principle, the symmetric representations of $O_4 \otimes O_4 \otimes S_2$ with $+$ sign are to be coupled to T_3^0 (parahelium), those with $-$ sign to T_3^1 (orthohelium). The results of the reductions are shown in Table I for parahelium and in Table II for orthohelium, with the respective spectroscopic signs in the right hand column.

Table I

n	Decomposition of Direct Products	Spectroscopic Signs
1	$T^{00+} \otimes T_3^0 = T_3^0 \otimes T_3^0 = T_+^0$	1^1S_0
2	$T^{10+} \otimes T_3^0 = (T_3^{0+} \oplus T_3^{1+}) \otimes T_3^0 = T_+^0 \oplus T_+^1$	2^1S_0, 2^1P_1
3	$T^{20+} \otimes T_3^0 = (T_3^{0+} \oplus T_3^{1+} \oplus T_3^{2+}) \otimes T_3^0 = T_+^0 \oplus T_+^1 \oplus T_+^2$	3^1S_0, 3^1P_0, 3^1D_2

In the case of $T^{k_1 0-}$ when $k_1 = 0$, the corresponding space is the zero vector, so we must begin with $k_1 = 1$, $n = 2$.

Table II

n	Decomposition of Direct Products	Spectroscopic Signs
2	$T^{10-} \otimes T_3^1 = (T_3^{0-} \oplus T_3^{1-}) \otimes T_3^1 = (T_3^{0-} \otimes T_3^1) \oplus (T_3^{1-} \otimes T_3^1) =$	
	$= T_-^1 \oplus$	2^3S_1
	$\oplus T_-^0 \oplus T_-^1 \oplus T_-^2$	2^3P_0, 2^3P_1, 2^3P_2
3	$T^{20-} \otimes T_3^1 = (T_3^{0-} \oplus T_3^{1-} \oplus T_3^{2-}) \otimes T_3^1 = (T_3^{0-} \otimes T_3^1) \oplus (T_3^{1-} \otimes T_3^1) \oplus$	
	$\oplus (T_3^{2-} \otimes T_3^1) = T_-^1 \oplus$	3^3S_1
	$\oplus T_-^0 \oplus T_-^1 \oplus T_-^2 \oplus$	3^3P_0, 3^3P_1, 3^3P_2
	$\oplus T_-^1 \oplus T_-^2 \oplus T_-^3$	3^3D_1, 3^3D_2, 3^3D_3

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ПРЕДСТАВЛЕНИЯ ГРУППЫ O_4 И СПЕКТРЫ ВОДОРОДА И ГЕЛИЯ

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Снова определена связь между некоторыми представлениями группы O_4 и уровнями водорода. Показаны особенности проявляющихся представлений. Состояния гелия могут быть получены также с помощью $O_4 \otimes O_4 \otimes S_2$.