GROUP THEORY OF THE KEPLER PROBLEM *

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The recent success of SU(6) symmetry in classifying elementary particles has triggered off a renewed interest in groups which are not invariance groups of dynamical systems but may yet be useful for characterizing the systems [1-3]. (By a group which is not an invariance group we mean one whose elements do not all commute with the Hamiltonian of the system.) One dynamical system which has been the focus of this renewed interest is the non-relativistic hydrogen atom, whose higher invariance group $O(4)$ is well-known, and for which a relevant non-invariant group, the De Sitter group $O(4,1)$ is also known †. In fact, in ref. 5, expressions for the generators of $O(4,1)$ in terms of the (classical) primitive dynamical variables have already been obtained explicitly.

The purpose of the present note is to investigate further the problem of the hydrogen atom from a group theoretical point of view, both in the classical and quantum mechanical cases. First, we interpret the arbitrary function and arbitrary parameter in the results of ref. 5. It turns out that the interpretation of the arbitrary parameter is non-trivial and leads to an important property of the group $O(4,1)$, namely that for arbitrary ν we can place the lowest ν levels of the atom in a representation of the corresponding compact group $O(5)$ and the remaining levels in a representation of $O(4,1)$, the matrix elements for the representation of the two groups being simple analytic continuations of one another. A second result we find is that there exists, besides $O(4,1)$, a second non-invariance group, namely SL(4, R), with similar properties, the difference being that whereas $O(4,1)$ classifies all energy levels, SL(4, R) classifies the even-numbered and odd-numbered levels separately, in Regge fashion. However, apart from $O(4,1)$ and SL(4, R), there are (in a sense to be explained) no other non-invariance groups. We find in addition that all our results generalize immediately to the case of the hydrogen atom in n dimensions. Finally, the positive and zero energy states, as well as the bound states, are investigated.

We now discuss these results more quantitatively. Letting p_r and q_r, $1 \leqslant r \leqslant n$ be the primitive dynamical variables in n dimensions, the hydrogen atom Hamiltonian

$$H = \tfrac{1}{2}p^2 - Z/q \,, \tag{1}$$

where

$$p^2 = \sum_{r=1}^{n} p_r^2 \,; \qquad q^2 = \sum_{r=1}^{n} q_r^2 \,; \qquad Z = \text{charge} \,, \tag{2}$$

has the angular momentum invariance group $O(n)$ with generator

$$q_r p_s - q_s p_r \tag{3}$$

and the higher invariance group (Fock-Bargman group) $O(n+1)$ with n extra (Lenz) generators

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† The exact origin of the knowledge that $O(4,1)$ is relevant is unknown to us.

$$A_k = (-2H)^{-\frac{1}{2}}\{Z(q\cdot p)p_k + (Z/q - p^2)q_k\} \qquad 1 \leqslant k \leqslant n \tag{4}$$

where

$$q\cdot p = \sum_{r=1}^{n} q_r p_r$$

It is understood that in the quantum mechanical case, the quantities occurring in eqs. (3) and (4) are to be appropriately symmetrized.

For positive energy it is clear from eq. (4) that the compact invariance group $O(n+1)$ changes to the non-compact form $O(n,1)$. For zero energy A_k is undefined, but if one uses instead $\overline{A_k} = \sqrt{-2H}\,A_k$ and then goes to the limit, one sees at once that the invariance group becomes E_n, the Euclidean group in n dimensions. From eq. (4) it is also clear that in the limiting case $Z = 0$, of a free particle, E_n is the relevant symmetry group.

For the negative energy case, the states of the νth-energy level furnish the symmetric tensor representation of rank ν of $O(n+1)$. With respect to the angular momentum group $O(n)$, this decomposes into a direct sum of symmetric tensor representations of rank $\mu = 0, 1, \ldots, \nu$, each one occurring once. The energy itself is given by

$$H = -\tfrac{1}{2}\{A^2 + L^2 + \tfrac{1}{4}(n-1)^2\}^{-1} \tag{5}$$

where

$$A^2 + L^2 = A_k A_k + \tfrac{1}{2}L_{jk}L_{jk}$$

is the Casimir operator of $O(n+1)$.

We can now go further and organize the lowest ν levels into a symmetric tensor representation of the non-invariance group $O(n+2)$, the remaining infinite number of levels constituting an irreducible unitary representation of the non-compact (generalized De Sitter) group $O(n+1,1)$.

In order to compute the extra generators needed to form the non-invariance groups $O(n+2)$ and $O(n+1,1)$, we follow Bacry [5] and restrict ourselves to the classical problem, using Poisson brackets instead of commutators. In the classical case, the non-invariance group transforms orbits with one energy into orbits with a different energy, while the invariance group generates transformations between orbits of the same energy. The explicit form of the generators are obtained by solving the differential equations entailed by the Poisson brackets. There are $n+1$ such generators and they transform like an $(n+1)$ vector with respect to $O(n+1)$, and an n-vector B_k, $k = 1, \ldots, n$, and a scalar S with respect to the angular momentum group $O(n)$. The general expressions for these vectors turn out to be

$$S = -\sqrt{\Lambda - 1/2H}\,\{(q\cdot p)\sqrt{-2H}\sin\psi + (qp^2 - 1)\cos\psi\}\,, \tag{6}$$

$$B_k = \sqrt{\Lambda - 1/2H}\{[q\sqrt{-2H}\cos\psi - (q\cdot p)\sin\psi]p_k + (1/q)\cos\psi\, q_k\}\,, \tag{7}$$

where

$$\psi = \{(q\cdot p)\sqrt{-2H} + \Theta(H)\} \tag{8}$$

and, for simplicity, we normalize Z to 1, since we are interested only in the case $Z \neq 0$. The solution thus depends on one arbitrary parameter Λ and an arbitrary function $\Theta(H)$. We can see, however, that the arbitrary function $\Theta(H)$ simply corresponds to the freedom to make a canonical transformation of the generators B_k and S by an arbitrary function of the Hamiltonian without altering the defining Poisson bracket relations; such a transformation would leave the generators of the invariance group $O(n+1)$ unaltered.

The parameter Λ is an essential parameter. For the negative energy orbits, for Λ positive, the expression $\Lambda - 1/2H$ is always positive. The $O(n+1,1)$ transformations thus generate transformations between all the closed orbits; distinct positive values of Λ correspond to inequivalent irreducible realizations of the transformation group. If we choose Λ to be negative, the $O(n+1,1)$ group is realized by the orbits with binding energy less than $1/2\Lambda$ (which is the binding energy of a circular orbit with radius $-\Lambda$). For orbits with larger binding energy, the generators B_k and S become pure imaginary. We could define a group $O(n+2)$ by choosing $B'_k = iB_k$ and $S' = iS$ as the additional generators; and then the $O(n+2)$ group would be realized irreducibly by transformations amongst these orbits.

Returining to the quantum mechanical case, we find that we have a similar situation, which we shall illustrate explicitly for $n = 3$, although it is true for all n. For $n = 3$ the Fock-Bargman invariance group is the group $O(4)$, and the states of the νth energy level furnish the symmetric tensor representation of rank ν of this group. Following the clue provided by the essential parameter Λ in the classical case, we look for an irreducible unitary representation of the non-invariance group $O(5)$ which will contain each of the states of the lowest ν energy levels of the atom just once (for arbitrary ν). It turns out that the symmetric tensor representation of rank ν of $O(5)$ has the required property. The problem of constructing this irreducible unitary representation of $O(5)$ explicitly clearly reduces to the problem of evaluating the reduced matrix elements of the extra generators B_k and S, $k = 1, 2, 3$ of $O(5)$, between the symmetric tensor states of $O(4)$. That is to say, if we let the states of each energy level (representation of $O(4)$) be labelled * as $|jjm_1m_2\rangle$, and define the reduced matrix element $\langle j'\|B\|j\rangle$ by

$$\langle j'j'm_1'm_2'|B^{\frac{1}{2}\,\frac{1}{2}}_{\mu_1\mu_2}|jjm_1m_2\rangle = C^{j\frac{1}{2}j'}_{m_1\mu_1m_1'}\,C^{j\frac{1}{2}j'}_{m_2\mu_2m_2'}\langle j'\|B\|j\rangle\,, \tag{9}$$

where $B^{\frac{1}{2}\frac{1}{2}}_{\mu_1\mu_2}$ is normalized so that

$$B^{\frac{1}{2}\frac{1}{2}}_{\frac{1}{2}-\frac{1}{2}} - B^{\frac{1}{2}\frac{1}{2}}_{-\frac{1}{2}\frac{1}{2}} = 2I_{54} \tag{10}$$

in the conventional notation, (and similarly for S), we find, using the explicit matrix elements of I_{54} found by Gelfand and Tseitlein [6], that, for $j' \neq j$, the only non-zero reduced matrix elements are essentially

$$\langle j+\tfrac{1}{2}\|B\|j\rangle = \frac{2j+1}{2j+2}\langle j\|B\|j+\tfrac{1}{2}\rangle = 2\sqrt{\frac{2j+1}{2j+2}}\sqrt{(\nu+1)^2 - (2j+1)^2} \tag{11}$$

with the restriction $2j \leqslant \nu$.

We then consider the remaining energy levels and look for an irreducible unitary representation of $O(4,1)$ which will contain these. We do not have to look very far because by making the simple transcription

$$\langle jj\|B'\|j+\tfrac{1}{2}\,j+\tfrac{1}{2}\rangle \rightarrow \langle jj\|\mathrm{i}B\|j+\tfrac{1}{2}\,j+\tfrac{1}{2}\rangle = \sqrt{\frac{(2j+1)^2 - (\nu+1)^2}{(2j+1)(2j+2)}}\,, \tag{12}$$

where $2j \geqslant \nu$, we obtain such an irreducible unitary representation. In particular for $\nu = -1$, we obtain an irreducible unitary representation of $O(4,1)$ which contains all the energy levels. Actually, in the latter case (*all* the energy levels) there exists even a one-parameter class of irreducible unitary representations of $O(4,1)$ into which they can be put. The class is obtained by setting $\nu = -1+\mathrm{i}\mu$ for any real μ in eq. (12).

Note that by the above procedure we not only establish the existence of an irreducible unitary representation of $O(5)$ which contains the lowest ν energy levels of the atom and one of $O(4,1)$ which contains the rest, but demonstrate that the matrix elements for those two are related by a simple process of analytic continuation. It might be worth mentioning that a similar property holds for other systems also [3].

For the (continuous) positive energy spectrum similar results can be obtained. We have already seen that in this case the Fock-Bargman invariance group is $O(n,1)$ and is therefore non-compact to begin with. From eqs. (6) and (7) it is clear that for Λ negative the non-invariance group is $O(n,2)$. For Λ positive, there exists an energy region ($H < 1/2\Lambda$) for which it is $O(n,2)$ and a region ($H > 1/2\Lambda$) for which it is $O(n+1,1)$. The last mentioned $O(n+1,1)$, however, is not the same $O(n+1,1)$ as in the negative energy case.

Having discussed the invariance groups $O(n+1)$ etc., and their containing non-invariance groups $O(n+2)$ and $O(n+1,1)$ etc., we come to the question as to whether these groups are unique.

First let us discuss the invariance group. It turns out that $O(n+1)$ is *not* the only group whose generators can be constructed out of the primitive variables and which contains the angular momentum group

* The general states of an irreducible unitary representation are labelled $|j_1j_2m_1m_2\rangle$ where j_1m_1 and j_2m_2 are the quantum numbers of the two $O(3)$'s in $O(4) = O(3)\times O(3)$. However, for symmetric tensor representations the second Casimir operator $C_2 = \epsilon^{abcd}J_{ab}J_{cd}$ is zero, with the result that $j_1 = j_2$. Hence the present labelling, with $j_1 = j_2 = j$. A further consequence of C_2 is that for the containing $O(5)$ or $O(4,1)$ the vector $\omega_f = \epsilon^{abcdf}J_{ab}J_{cd}$ is zero, since it can be generated from $\omega_5 = C_2$. Hence the Casimir operator $\omega_f\omega^f$ of $O(5)$ or $O(4,1)$ is zero. Thus for $O(5)$ of $O(4,1)$ also, only one label is necessary for the relevant irreducible unitary representations.

and commutes with the Hamiltonian. The group SU(n) also has these properties. The extra generators required to extend $O(n)$ to SU(n) from a second rank traceless symmetric tensor with respect to $O(n)$, and can easily be constructed from the Lenz vector. For example, if in the 3-dimensional case we denote this tensor by Q_2^m, m = -2, -1.0, 1, 2, we obtain

$$Q_2^2 = A_1' f(J^2) A_1' + g(J^2) J_1'^2 , \tag{13}$$

where

$$f[(l+1)(l+2)] = \sqrt{2(2l+1)} \sqrt{\frac{\lambda(\lambda+3) - l(l+3)}{[(\mu+1)^2 - (l+1)^2][(\mu+1)^2 - (l+2)^2]}} ,$$

$$\frac{g[l(l+1)]}{\sqrt{2}} = -\frac{(2\lambda+3)}{(2l-1)(2l+3)} + \frac{1}{\sqrt{2l+1}\,(2l+3)} \sqrt{\frac{[\lambda(\lambda+3) - l(l+3)][(\mu+1)^2 - (l+1)^2]}{(\mu+1)^2 - (l+2)^2}} + \frac{1}{\sqrt{2l-1}} \frac{1}{2l+1} \sqrt{\frac{[\lambda(\lambda+3) - (l-2)(l+1)][(\mu+1)^2 - l^2]}{[(\mu+1)^2 - (l-1)^2]}} \tag{14}$$

J^2 is the total angular momentum, and A is the Lenz vector defined in (4) and $\lambda = n - \frac{1}{2}(1 - P(-)^n)$, where P is the parity operator $(-1)^J$ and n is defined by $H = -1/2n^2$. Unlike $O(n+1)$, the symmetric tensor representations of SU(n) do not contain every state in a given energy level of the atom, but only every state with *even* angular momentum (or alternatively every state with *odd* angular momentum). In this sense SU(n) is less comprehensive than $O(n+1)$. On the other hand, this property of SU(n) is a consequence of the fact that, unlike $O(n+1)$, it commutes with the parity operator.

For positive energies we have seen that the invariance group $O(n+1)$ becomes $O(n, 1)$. Similarly one can verify that for positive energies SU(n) becomes SL(n, R). The unitary irreducible representations of SL(n, R) obtained by making the analytic continuation

$$\lambda \to -\tfrac{3}{2} + i\sigma , \qquad \sigma \text{ real} \tag{15}$$

in (14), contains all the even (or odd) angular momentum states for any given positive value of H.

We turn now to the case of the non-invariance groups. For negative energies the non-invariance groups used above were $O(n+2)$ and $O(n+1, 1)$. It turns out that, just as in the case of the invariance groups these groups are not unique. The groups SU($n+1$) and SL($n+1$, R) have similar properties. The properties of SU($n+1$) and SL($n+1$, R) differ from those of $O(n+2)$ and $O(n+1, 1)$ in two respects however: 1) $O(n+2)$ gathers together the lowest ν levels of the atom for arbitrary ν, whereas, as might be expected from the discussion of the invariance groups above, SU($n+1$) gathers together only the lowest ν *even*-numbered (or odd-numbered) levels. 2) For a given ν, there exists an analytic continuation of the irreducible unitary representation of $O(n+2)$ containing the first ν levels, which gives an irreducible unitary representation of $O(n+1, 1)$ containing all the *remaining* levels. But the analytic continuation of the irreducible unitary representation of SU($n+1$) containing the first ν even (or odd) levels yields one of SL($n+1$, R) which contains *all* the even (or odd) levels of the atom.

In these two senses the set {SU($n+1$), SL($n+1$, R)} is less comprehensive than the set {$O(n+2)$, $O(n+1, 1)$}. However, in a sense the set {SU($n+1$), SL($n+1$, R)} is more characteristic of the dynamical system since on account of (b) it demands the existence of all the energy levels that actually occur.

Having discovered a group other than $O(n+2)$ or $O(n+1, 1)$ one might ask next whether any further groups of this kind exist, or whether $O(n+2)$ and SU($n+1$) are in any sense unique. It is easy to prove that they are unique in the following sense at any rate. $O(n+2)$ is the only simple group which, for arbitrary ν, can group together the ν lowest energy levels of the atom, and SU($n+1$,) is the only group which, for arbitrary ν can group the ν lowest even (or odd) levels. Further, there is no group with an irreducible unitary representation containing every 3rd, 4th, ... level up to any energy.

The question as to what becomes of SU($n+1$) and SL($n+1$, R) when the energy becomes positive is somewhat complicated and will not be discussed here.

In conclusion we might mention that besides asking the question as to whether the groups $O(4)$, $O(4, 1)$ etc., are unique, one might ask the question: given the group, are the irreducible unitary representation of it which we have used unique or are there other ones which are relevant for this problem. It turns out that for $O(n+1)$, for example, the symmetric tensor representations are not the only relevant ones. There exist other representations which contain instead of the angular momentum states in the range $0 \leqslant l \leqslant \nu$, those in the range $\mu \leqslant l \leqslant \nu$, for arbitrary μ and ν. The matrix elements of these irreducible unitary representations can also be analytically continued and yield one of $O(4,1)$ which contains all the states for which $l \geqslant \mu$. We shall not exhibit these matrix elements as an analogous set have been exhibited elsewhere [3]. It is, perhaps, interesting to note that for the other invariance group, SU(n), no such irreducible unitary representations exist, the symmetric tensor representations are unique.

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