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O(3, 1) symmetry of the hydrogen atom

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Abstract. The transformation coefficients connecting the Stark and the angular momentum states belonging to the positive spectrum of the hydrogen atom are calculated by a group-theoretical method which makes use of the O(3, 1) symmetry of the states and also by a purely analytical method. The results of the two calculations agree except for an undetermined factor not containing the orbital quantum number l. Complete agreement between the results is achieved by taking the normalization factors for the continuum states to be analytic continuations of those for the bound states. The transformation coefficients turn out to be SU(2) Clebsch–Gordan coefficients $(j_1 j_2 l : m_1 m_2 m)$ with complex $j_1 j_2 m_1 m_2$, and physical l, m. From the general theory the well known expansion of the Coulomb scattering function is obtained by giving the magnetic quantum number m and one of the electric quantum numbers, n_2, the special values, 0 and -1, respectively.

1. Introduction

It is well known (Lenz 1924, Pauli 1926, Bargmann 1936) that, in the case of the non-relativistic hydrogen atom, there is an additional operator

$$M = (2\mu)^{-1}(\boldsymbol{p}\times\boldsymbol{L}-\boldsymbol{L}\times\boldsymbol{p})-Ze^2\frac{\boldsymbol{r}}{r}$$

which commutes with the hamiltonian $H = (2\mu)^{-1}p^2-Ze^2/r$. In a fixed energy subspace $\boldsymbol{L}$ and $\boldsymbol{M}$ satisfy the commutation relations,

$$[L_i, L_j] = \mathrm{i}\epsilon_{ijk}L_k, \qquad [L_i, M_j] = \mathrm{i}\epsilon_{ijk}M_k$$
$$[M_i, M_j] = -\mathrm{i}\frac{2E}{\mu}\epsilon_{ijk}L_k. \tag{1.1}$$

When $\boldsymbol{M}$ is replaced by $\hat{\boldsymbol{M}} = (\mu/e|E|)^{1/2}\boldsymbol{M}$, these become the commutation relations for the generators of O(4) if $E < 0$ and O(3, 1) if $E > 0$. The bound and the scattering states of the hydrogen atom, therefore, form bases of irreducible representations of O(4) and O(3, 1), respectively. The O(4) symmetry of the bound states has been investigated in great detail by a number of authors (Fock 1935, Park 1960, Bethe and Leon 1962, Swamy and Biedenharn 1964, Dothan *et al* 1965, Sudarshan *et al* 1965, Barut *et al* 1966, Flamand 1966, Bander and Itzykson 1966, Hughes 1967, Joseph 1967, Barut and Kleinert 1967) and the main results that have emerged are the following:

(i) The irreducible representations of O(4) that occur in the problem are of the special type $D^{j_1 j_2}$ with $j_1 = j_2 = \frac{1}{2}(n-1)$.

(ii) For the same energy, the angular momentum states ψ_{nlm} and the Stark states $\psi_{n_1n_2m}$ constitute different bases of the same irreducible representation, and the transformation coefficients connecting them are SU(2) Clebsch–Gordan coefficients (CGC).

In the present paper we shall show that the results established for the bound states hold also for the scattering states provided we allow certain quantities to take unphysical complex values. The relation, $j_1 = j_2 = \frac{1}{2}(n-1)$, again holds with imaginary n and complex j_1, j_2, and the transformation coefficients between the angular momentum and the Stark states turn out to be complex generalizations of the SU(2) CGC. In fact, it is found that, with a proper interpretation of the mathematical symbols, the same theory applies to the bound and the scattering states. This was demonstrated in Basu and Majumdar (1973, to be referred to as I) for the special case of Coulomb scattering of an electron by a positively charged centre. We consider this problem again in the present paper for clarifying certain points and then pass on to the general case.

2. The case of Coulomb scattering

In order to test the correctness of conclusion (ii) above in the case of scattering states the well known expansion of the Coulomb scattering function

$$\phi_c = e^{ikz}\,{}_1F_1(-iN, 1, ik(r-z)) \tag{2.1}$$

with

$$N = \frac{-Ze^2}{\hbar}\left(\frac{\mu}{2E}\right)^{1/2}, \qquad k = \left(\frac{2\mu E}{\hbar^2}\right)^{1/2}$$

was rederived in I by the group-theoretical method. Operated on by $\frac{1}{2}(\boldsymbol{L} \pm i\hat{\boldsymbol{M}})$, ϕ_c was found to behave like the product $\psi_{j_1m_1}\psi_{j_2m_2}$ with $j_1 = j_2 = -m_1 = m_2 = \frac{1}{2}(n-1)$. Consequently, the expansion of ϕ_c in terms of the angular momentum states $\psi_{nl0} = N_{nl0}\phi_{nl0}$ took the form

$$\phi_c = \sum_l \{\tfrac{1}{2}(n-1), \tfrac{1}{2}(n-1), l: -\tfrac{1}{2}(n-1), \tfrac{1}{2}(n-1), 0\} N_{nl0}\rho^l e^{-\rho/2} \times {}_1F_1(1+l-n, 2l+2; \rho) P_l(\cos\theta) \tag{2.2}$$

with $n = -iN$, $\rho = -2ikr$, and the curly brackets denoting a CGC. With appropriate values of N_{nl0} this was found to be in agreement with the standard expansion. To demonstrate this we determine the 'normalization factors' of the wavefunctions ψ_{nl0} of the continuous spectrum. This we do by using the hermitian property of $\hat{M}_3$. By definition,

$$\hat{M}_3 = (2\hbar k)^{-1}(\boldsymbol{p} \times \boldsymbol{L} - \boldsymbol{L} \times \boldsymbol{p})_3 + i\hbar n u, \tag{2.3}$$

where

$$u = \cos\theta.$$

Since the functions on which it operates are independent of ϕ, $\hat{M}_3$ is effectively equal to

$$2i\hbar\left[(u^2-1)\frac{\partial^2}{\partial\rho\,\partial u} + u\left(\frac{\partial}{\partial\rho} - \frac{l(l+1)}{\rho}\right)\right] + i\hbar n u.$$

Operating on ϕ_{nl0} this gives

$$\hat{M}_3\phi_{nl0} = -2i\hbar l^2\phi_{nl-10} + i\hbar\frac{(1+l-n)(1+l+n)}{2(2l+1)(2l+3)}\phi_{nl+10}. \tag{2.4}$$

The result is obtained by using the recursion relations for $P_l(u)$ and the relations

$$F(a,c) - F(a+1,c+1) = \frac{a-c}{c(c+1)}\rho F(a+1,c+2) \tag{2.5}$$

$$F(a,c) + \frac{a-c+1}{(c-1)(c-2)}\rho F(a,c) + \frac{a}{c(c-1)}\rho F(a+1,c+1) = F(a-1,c-2), \tag{2.6}$$

where $F(a,c)$ denotes ${}_1F_1(a,c;\rho)$. The hermiticity of $\hat{M}_3$ now gives

$$\left|\frac{N_{nl0}}{N_{nl-10}}\right|^2 = \frac{(l-n)(l+n)}{4l^2(2l-1)(2l+1)} \tag{2.7}$$

whence,

$$\left|\frac{N_{nl0}}{N_{n00}}\right|^2 = \frac{\Gamma(1+l-n)\Gamma(1+l+n)}{\Gamma(1-n)\Gamma(1+n)(2l)!(2l+1)!} \tag{2.8}$$

$$\langle n\, l+1\, 0|\hat{M}_3|n\, l\, 0\rangle = i\hbar(l+1)\left(\frac{(1+l-n)(1+l+n)}{(2l+1)(2l+3)}\right)^{1/2} \times \text{phase factor}. \tag{2.9}$$

The expression (2.8), substituted in (2.2), gives the standard expansion of ϕ_c except for an undetermined factor occurring outside the summation.

The treatment given above of the Coulomb scattering case cannot be regarded as wholly satisfactory. For, the method delineated here does not determine the normalization factor N_{n00}. Secondly, the function ϕ_c does not seem to have any connection with the general Stark state of the continuum. These shortcomings will be removed in the next section by using the concept of analyticity.

3. The general Stark state of the continuous spectrum

As already indicated, the general Stark state $\psi_{n_1n_2m}$ of the continuum may be regarded as an analytic continuation, in both parameters and variables, of the bound state

$$\psi_{n_1n_2m} = N'_{n_1n_2m}(2p_0r)^{|m|}\sin^{|m|}\theta\, e^{-p_0r}\, e^{im\phi} \times {}_1F_1(-n_1,|m|+1;2p_0r\mu)\,{}_1F_1(-n_2,|m|+1;2p_0r\lambda) \tag{3.1}$$

with

$$\lambda = \tfrac{1}{2}(1-\cos\theta), \qquad \mu = \tfrac{1}{2}(1+\cos\theta)$$

$$N'_{n_1n_2m} = p_0^{3/2}2^{-m}\left(\frac{\Gamma(n_1+m+1)\Gamma(n_2+m+1)}{\Gamma(n_1+1)\Gamma(n_2+1)(m!)^4\pi n}\right)^{1/2} \tag{3.2}$$

$$n_1+n_2+|m|+1 = n. \tag{3.3}$$

In the case of scattering states, n_1 and n_2 are arbitrary complex numbers subject to the restriction (3.3) with integral m and imaginary n. The angular momentum states ψ_{nlm}

of the continuum are, likewise, analytic continuations of the states

$$\psi_{nlm} = N'_{nlm}\, e^{-p_0 r}(2p_0 r)^l {}_1F_1(1+l-n, 2l+2; 2p_0 r) P_l^m(\cos\theta)\, e^{im\phi} \tag{3.4}$$

with

$$N'_{nlm} = \frac{(-1)^m p_0^{3/2}}{(2l+1)!}\left(\frac{\Gamma(n+l+1)(l-m)!(2l+1)}{\Gamma(n-l)(l+m)!\pi n}\right)^{1/2}.$$

The analytic continuation is performed by putting

$$\rho = 2p_0 r, \qquad p_0 = \left(\frac{-2\mu E}{\hbar^2}\right)^{1/2} = -ik, \qquad n = -iN, \qquad k > 0, N < 0. \tag{3.5}$$

For complex n_1, n_2 and imaginary n the function $\psi_{n_1 n_2 m}$ is, therefore, expected to admit an expansion in terms of the functions ψ_{nlm}, the coefficients in the expansion being analytic continuations of SU(2) CGC. This implies the existence of an identity of the type

$$\rho^{|m|}(1-u^2)^{|m|/2} {}_1F_1(a, c; \lambda\rho) {}_1F_1(a', c; \mu\rho) = \sum_{l=|m|}^{\infty} \beta_l \rho^l {}_1F_1(a+a'+l-|m|, 2l+2; \rho) P_l^m(\cos\theta) \tag{3.6}$$

with $c = |m|+1$. The expansion of $\psi_{n_1 n_2 m}$ in terms of ψ_{nlm} is obtained on multiplying both sides by $\exp[i(m\phi + kr)]$. We now proceed to establish this identity by the standard methods of analysis taking c to be a positive integer and a, a' to be arbitrary complex numbers.

Denoting the left-hand side of (3.6) by L and expanding the angular part in a series of Legendre functions, we have, for $m \geqslant 0$,

$$L = \frac{\{\Gamma(c)\}^2}{\Gamma(a)\Gamma(a')} \sum_{n=m}^{\infty} \sum_{r=0}^{n-m} 2^{-n+m} \rho^n \frac{\Gamma(a+r)\Gamma(a'+n-m-r)}{(m+r)!(n-r)!r!(n-m-r)!} f(u) \tag{3.7}$$

$$f(u) = (1-u)^{r+m/2}(1+u)^{n-r-m/2} = \sum_l (-1)^m 2^n \frac{(m+r)!(n-r)!(2l+1)}{m!(n+m+1)!} {}_3F_2\left[\begin{matrix} -l+m, l+m+1, r+m+1; \\ m+n+2, m+1 \end{matrix}\right] P_l^m(u), \tag{3.8}$$

where, ${}_3F_2[\ ]$ denotes a generalized hypergeometric series of unit argument. The identity (Bailey 1935, Slater 1966)

$${}_3F_2\left[\begin{matrix} a, b, c; \\ d, e \end{matrix}\right] = \frac{\Gamma(d)\Gamma(d-a-b)}{\Gamma(d-a)\Gamma(d-b)} {}_3F_2\left[\begin{matrix} a, b, e-c; \\ a+b-d+1, e \end{matrix}\right] + \frac{\Gamma(d)\Gamma(e)\Gamma(a+b-d)\Gamma(d+e-a-b-c)}{\Gamma(a)\Gamma(b)\Gamma(e-c)\Gamma(d+e-a-b)} \times {}_3F_2\left[\begin{matrix} d-a, d-b, d+e-a-b-c; \\ d-a-b+1, d+e-a-b \end{matrix}\right] \tag{3.9}$$

then gives,

$$f(u)=\frac{(-1)^m 2^n}{m!}\sum_{l=m}^{n}\frac{(m+r)!(n-r)!(n-m)!(2l+1)}{(n+l+1)!(n-l)!}\,{}_3F_2\left[\begin{matrix}-l+m,\, l+m+1,\, -r\,;\\ -n+m,\, m+1\end{matrix}\right]P_l^m(u). \tag{3.10}$$

When (3.10) is substituted in (3.7) and the ${}_3F_2(1)$ series is written in an expanded form with s as the summation index, $r!$ cancels out from the numerator and the denominator and the sum over r reduces to a ${}_2F_1(1)$ series. This ${}_2F_1(1)$ series can be evaluated by using Gauss's formula, ${}_2F_1(a,b\,;c\,;1)=\Gamma(c)\Gamma(c-a-b)/\Gamma(c-a)\Gamma(c-b)$. When this is done, the sum over s reduces to another ${}_3F_2(1)$ series and L takes the form

$$L=\frac{(-1)^m 2^m m!}{\Gamma(a+a')}\sum_{l=m}^{\infty}(2l+1)\,{}_3F_2\left[\begin{matrix}-l+m,\, l+m+1,\, a\,;\\ a+a',\, m+1\end{matrix}\right]\sum_{t=0}^{\infty}\rho^{l+t}\frac{\Gamma(a+a'+l-m+t)}{\Gamma(2l+2+t)t!}P_l^m(u) \tag{3.11}$$

with

$$n=l+t.$$

From (3.11) it is evident that the identity (3.6) holds with

$$B_l=\frac{(-1)^m 2^m m!\,\Gamma(a+a'+l-m)}{\Gamma(a+a')(2l!)}\,{}_3F_2\left[\begin{matrix}-l+m,\, l+m+1,\, a\,;\\ a+a',\, m+1\end{matrix}\right] \tag{3.12}$$

and with no restriction imposed on a, a'.

If conclusion (ii) of the introduction is correct the expression (3.12) for B_l must be a multiple of the complex CGC $\{j_1 j_2 l : m_1 m_2 m\}$ with

$$j_1=j_2=\tfrac{1}{2}(n-1)=\tfrac{1}{2}(-a-a'+m) \tag{3.13}$$

$$m_1=\tfrac{1}{2}(-a+a'+m), \qquad m_2=\tfrac{1}{2}(a-a'+m)$$

and l, m physical. These values are obtained by applying the operators $\tfrac{1}{2}(\boldsymbol{L}\pm\mathrm{i}\hat{\boldsymbol{M}})$ to $\phi_{aa'm}$. In the search for a suitable expression for the CGC (Yutsis *et al* 1962) it has been observed that the various expressions available in the literature do not always give the same result when the j's and the m's take complex values. A similar situation arises in the case of the CGC of SU(1, 1). Some caution is, therefore, necessary in using such expressions for evaluating a complex CGC. In the present case the desired result is obtained by taking

$$\begin{aligned}\{j_1 j_2 j : m_1 m_2 m\} &= (-1)^{j_1-j+m_2}(2j+1)^{1/2}\\ &\times\left(\frac{\Gamma(j_1+j_2-j+1)\Gamma(j_1-j_2+j+1)\Gamma(-j_1+j_2+j+1)}{\Gamma(j_1+j_2+j+2)}\right)^{1/2}\\ &\times\left(\frac{\Gamma(j+m+1)\Gamma(j_2+m_2+1)\Gamma(j_1+m_1+1)\Gamma(j_1-m_1+1)}{\Gamma(j-m+1)\Gamma(j_2-m_2+1)}\right)^{1/2}\\ &\times\frac{1}{\Gamma(j_1-j_2+m+1)\Gamma(j_1-j+m_2+1)}\\ &\times\frac{1}{\Gamma(j+j_2-j_1+1)}\,{}_3F_2\left[\begin{matrix}-j+m,\, -j_2+m_2,\, -j-j_2+j_1\,;\\ j_1-j+m_2+1,\, j_1-j_2+m+1\end{matrix}\right].\end{aligned} \tag{3.14}$$

When the values (3.13) and the identity (3.9) are used, this reduces to

$$\mathrm{CGC} = (-1)^{j_1-j+m_2}\left(\frac{(2l+1)(l+m)!\,\Gamma(j_1+m_1+1)\Gamma(j_2+m_2+1)}{(l-m)!\,\Gamma(j_1-m_1+1)\Gamma(j_2-m_2+1)\Gamma(2j_1+l+2)\Gamma(2j_1-l+1)}\right)^{1/2}$$

$$\times\frac{\Gamma(2j_1-m+1)}{m!}\,{}_3F_2\left[\begin{matrix}-l+m,\, l+m+1,\, a;\\ a+a',\, m+1\end{matrix}\right]. \tag{3.15}$$

In this form the CGC has a strong resemblance to the expression (3.12) for B_l. The product of the CGC and the normalization factor N_{nlm} determined by the method of § 2 is

$$\frac{\Gamma(1+l-n)}{(2l)!}\,{}_3F_2\left[\begin{matrix}-l+m,\, l+m+1,\, a;\\ a+a',\, m+1\end{matrix}\right],$$

and this is identical with the l-dependent part of B_l.

It is interesting to note that the normalization factor N_{nlm} obtained by the group-theoretical method differs trivially from the analytic continuation of the factor N'_{nlm} of equation (3.4). The same is found to be true of $N'_{n_1n_2m}$ and $N_{n_1n_2m}$ if the latter is determined by applying the raising and lowering operators $\frac{1}{2}(\boldsymbol{L}\pm \mathrm{i}\hat{\boldsymbol{M}})$ to the state $\psi_{n_1n_2m}$ of the continuum. It will therefore be legitimate to use the primed N as the normalization factors of the continuum states. When this is done the coefficients $B_lN'_{aa'm}/N'_{nlm}$ in the expansion become identical with the CGC (3.15).

We conclude with a remark on the Coulomb scattering case discussed earlier. For $m=0$, $a=-n$, $a'=1$, one of the ${}_1F_1$-functions in (3.6) reduces to $\exp[-\mathrm{i}k(r+z)]$ and the ${}_3F_2(1)$ series in (3.12) becomes saalschützian. The expansion of ϕ_{-n10} then takes the form

$$\mathrm{e}^{-\mathrm{i}kz}\,{}_1F_1(\mathrm{i}N, 1; -\mathrm{i}k(r-z))$$

$$=\frac{\mathrm{e}^{\mathrm{i}kr}}{\Gamma(-\mathrm{i}N+1)}\sum_{l=0}^{\infty}\frac{\Gamma(l-\mathrm{i}N+1)}{\Gamma(2l+1)}(-2\mathrm{i}kr)^l$$

$$\times\,{}_1F_1(l+1+\mathrm{i}N, 2l+2; -2\mathrm{i}kr)P_l(\cos\theta). \tag{3.16}$$

From this the standard expansion of ϕ_c is obtained by using the identity,

$${}_1F_1(1+l-n, 2l+2; \rho) = \mathrm{e}^{\rho}\,{}_1F_1(1+l+n, 2l+2; -\rho) \tag{3.17}$$

and taking the complex conjugate of both sides.

References

Bailey W N 1935 *Generalized Hypergeometric Series* (London: Cambridge University Press)
Bander M and Itzykson C 1966 *Rev. mod. Phys.* **38** I 330 II 346
Bargmann V 1936 *Z. Phys.* **99** 576
Barut A O, Budini P and Fronsdal C 1966 *Proc. R. Soc.* A **291** 106
Barut A O and Kleinert H 1967 *Phys. Rev.* **160** 1149
Basu D and Majumdar S D 1973 *J. Phys.* A: *Math., Nucl. Gen.* **6** 1097
Bethe H A and Leon M 1962 *Phys. Rev.* **127** 636
Dothan Y, Gell-Mann M and Neeman Y 1965 *Phys. Rev. Lett.* **17** 148
Flamand G 1966 *J. math. Phys.* **7** 1924
Fock V 1935 *Z. Phys.* **98** 145
Hughes J W B 1967 *Proc. Phys. Soc.* **91** 810
Joseph A 1967 *Rev. mod. Phys.* **39** 829

Lenz W 1924 *Z. Phys.* **24** 197
Park D 1960 *Z. Phys.* **159** 155
Pauli W 1926 *Z. Phys.* **36** 336
Slater L J 1966 *Generalized Hypergeometric Functions* (London: Cambridge University Press)
Sudarshan E C G, Mukunda N and O'Raifeartaigh L 1965 *Phys. Rev. Lett.* **19** 322
Swamy N V V J and Biedenharn L C 1964 *Phys. Rev.* **133** B1353
Yutsis A P, Levinson I B and Vanagas V V 1962 *Mathematical Apparatus of the Theory of Angular Momentum* (Jerusalem: *Israel Program for Scientific Translations*)