

ON THE "HIDDEN" SYMMETRY OF THE HYDROGEN ATOM

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A number of problems related to the so-called "hidden" symmetry of the hydrogen atom are considered. The wave functions of the discrete spectrum are written as polynomials of the two complex variables z_1 and z_2 in analogy to the Fock-Bargmann representation for the harmonic oscillator. It is shown that the wave functions of the continuous spectrum of the hydrogen atom can be used to set up generalized "representations" of the rotation group corresponding to complex values of the angular momentum $j = -\frac{1}{2} + i\rho$ ($-\infty < \rho < \infty$). The expansion of the direct product of these representations is considered, and it is shown that this expansion involves the usual (integer) values of the angular momentum. The corresponding Clebsch-Gordan coefficients are given in terms of the Coulomb scattering phase.

THE nonrelativistic hydrogen atom has a specific degeneracy (independence of the energy $E_{nl} = -1/2n^2$ on the orbital angular momentum l) which has received the name "accidental degeneracy." This feature was explained in a known paper of Fock^[1] (cf. also^[2]) who showed that the Hamiltonian of the hydrogen atom is invariant with respect to the group $O(4)$ (higher symmetry group). Subsequently, this symmetry has been studied more closely,^[3-8] in particular, for the states of the continuous spectrum^[5,6] and in the n -dimensional case.^[3,4,6,8]

In the present paper we consider a number of problems related to the "accidental" degeneracy in a Coulomb field. In Sec. 1 we construct the simplest realization of the bound states of the hydrogen atom in analogy to the known Fock-Bargmann representation for the harmonic oscillator.^[9,10] The transition to the case of positive energies allows one to consider the coupling of two complex angular momenta (of the special form $j_1 = j_2 = -\frac{1}{2} + i\rho$) and to find the corresponding Clebsch-Gordan coefficient. It turns out that it can be expressed through the Coulomb scattering phase (Sec. 2).

1. WAVE FUNCTIONS OF THE DISCRETE SPECTRUM IN THE z REPRESENTATION

Evidently, the simplest of the possible realizations of the operators a and a^+ for the harmonic oscillator is the so-called Fock-Bargmann representation;^[9,10] it has proved convenient for the solution of a number of problems,^[11] in particular those related to the account of the "hidden" symmetry of the harmonic oscillator. Below we construct an analogous realization for the wave functions of the hydrogen atom.

As is known,^[2,4] the symmetry group of the Coulomb potential $V(r) = -\alpha/r$ is generated by the integrals of motion—the angular momentum L and the Runge-Lenz vector A :

$$A = n + \frac{1}{2m\alpha} \{[Lp] - [pL]\}, \quad n = r/r. \tag{1}^*$$

Going over to the operators

$$J_{1,2} = \frac{1}{2}(L \pm M), \quad M = (-2H)^{-1/2}A, \tag{2}$$

* $[Lp] \equiv L \times p$.

we obtain

$$[J_1, J_1] = iJ_1, \quad [J_2, J_2] = iJ_2, \quad [J_1, J_2] = 0, \tag{3}$$

$$J_1^2 = J_2^2 = \frac{1}{4}(L^2 + M^2) = -\frac{1}{4}(1 + \frac{1}{2}H^{-1}), \tag{4}$$

where $H = p^2/2 - 1/r$ (in atomic units). A representation in which J_{1z} and J_{2z} are diagonal is realized by wave functions in parabolic coordinates.^[2,6] Indeed,

$$L_z \psi_{n_1, n_2, m} = m \psi_{n_1, n_2, m}, \quad A_z \psi_{n_1, n_2, m} = \frac{n_1 - n_2}{n} \psi_{n_1, n_2, m}, \tag{5}$$

$$J_{1z} \psi_{n_1, n_2, m} = \mu_1 \psi_{n_1, n_2, m}, \quad \mu_1 = \frac{1}{2}(m + n_1 - n_2), \quad \mu_2 = \frac{1}{2}(m - n_1 + n_2). \tag{6}$$

Here n_1 and n_2 are the parabolic quantum numbers, cf.^[12]; $n_1 + n_2 + |m| = n - 1$ (our definition of the vector A differs from that of^[12] by a sign).

We recall how the irreducible representation with weight j of the group $SU(2)$ is constructed in the z plane.^[13] The transformation of the wave functions under spatial rotations is given by the formula

$$T_{uf}(z) = (\beta z + \delta)^{2j} f\left(\frac{\alpha z + \gamma}{\beta z + \delta}\right), \tag{7}$$

where

$$u = \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix} \quad \begin{aligned} \alpha &= \delta^* = e^{-i(\psi+\varphi)/2} \cos(\theta/2) \\ \beta &= -\gamma^* = -ie^{-i(\psi-\varphi)/2} \sin(\theta/2) \end{aligned} \tag{8}$$

(ψ, θ, φ are the Euler angles). The scalar product which is invariant under (7) has the form

$$(f, g) = \int d\mu_j(z) f^*(z) g(z), \tag{9}$$

where

$$d\mu_j(z) = \frac{2j+1}{\pi} \frac{dz}{(1+|z|^2)^{2j+2}}; \quad \int d\mu_j(z) = 1 \tag{10}$$

[the integration in (10) goes over the whole z plane: $dz = dx dy, -\infty < x, y < \infty$]. Going over to the case $u \rightarrow 1$ in (7), we find the generators

$$J_+ = -z^2 \frac{d}{dz} + 2jz, \quad J_0 = z \frac{d}{dz} - j, \quad J_- = \frac{d}{dz} \tag{11}$$

($J_{\pm} = J_x \pm iJ_y, J_0 = J_z$). The operators J_+ and J_0 of this realization depend on the value of the angular momentum j . The states $|jm\rangle$ are represented by the terms

$$|jm\rangle = f_{jm}(z) = \left[\frac{(2j)!}{(j+m)!(j-m)!} \right]^{1/2} z^{j+m}. \tag{12}$$

The functions $f_{jm}(z)$ are orthogonal and normalized in the sense (10), and the generators J_μ act on them according to the usual formulas of quantum mechanics:

$$J_\pm |jm\rangle = [(j \mp m)(j + 1 \pm m)]^{1/2} |j, m \pm 1\rangle, J_0 |jm\rangle = m |jm\rangle. \quad (13)$$

Let us now introduce the two complex variables z_1 and z_2 corresponding to the operators J_1 and J_2 of (3). Then, in accordance with (6) and (12), the state $|n_1 n_2 m\rangle$ of the hydrogen atom is written

$$\begin{aligned} |n_1 n_2 m\rangle &= f_{j\mu_1}(z_1) f_{j\mu_2}(z_2) \\ &= \frac{(n-1)!}{[n_1! n_2! (n_1 + |m|)! (n_2 + |m|)!]^{1/2}} z_1^{n_1 + (m+|m|)/2} z_2^{n_2 + (m+|m|)/2}, \end{aligned} \quad (14)$$

where $j = (n - 1)/2$. Let us determine the wave functions of the states $|nlm\rangle$ with definite orbital angular momentum. Since $L = J_1 + J_2$ and $[J_1, J_2] = 0$, this problem is equivalent to the coupling of two angular momenta. The basis in the space of the reducible representation $D_{j_1} \otimes D_{j_2}$ is provided by the set of terms $f_{j_1 \mu_1}(z_1) f_{j_2 \mu_2}(z_2)$.

The expansion into irreducible representations can be found by the following consideration. In the space of each irreducible representation D_j there is a lowest vector $|j, -j\rangle$ for which $L_- |j, -j\rangle = 0$. Since $L_- = \partial/\partial z_1 + \partial/\partial z_2$ [cf. (11)], then $f_{j, -j}(z_1, z_2) = N(z_1 - z_2)^{j_1 + j_2 - j}$, where N is a normalization constant. Acting on $f_{j, -j}$ with the operators L_+ , one can find all remaining vectors f_{jm} . These calculations are easily carried out for arbitrary values of j_1 and j_2 ; we give the answer for the special case of interest to us, $j_1 = j_2 = (n - 1)/2$:

$$\psi_{nlm}(z_1, z_2) = A_{nl}(z_1 - z_2)^{n-l-1} \Pi_{lm}(z_1, z_2), \quad (15)$$

where

$$\begin{aligned} A_{nl} &= \frac{(n-1)!}{l!} \left[\frac{(2l+1)!}{(n+l)!(n-l-1)!} \right]^{1/2}, \\ \Pi_{lm}(z_1, z_2) &= \left[\frac{(l+m)!}{(2l)!(l-m)!} \right]^{1/2} \left(\frac{\partial}{\partial z_1} + \frac{\partial}{\partial z_2} \right)^{l-m} (z_1 z_2)^l \\ &= \left[\frac{(l+m)!(l-m)!}{(2l)!} \right]^{1/2} \sum_{k=0}^{l+m} C_l^k C_l^{k-m} z_1^k z_2^{l+m-k}. \end{aligned} \quad (16)$$

Thus $\psi_{nlm}(z_1, z_2)$ is a homogeneous polynomial of degree $n + m - 1$. The summation in (16) is actually restricted by the condition

$$\min(l, l+m) \geq k \geq \max(0, m), \quad (17)$$

so that the polynomial $\Pi_{lm}(z_1, z_2)$ consists of $(l + 1 - |m|)$ terms. In particular,

$$\Pi_{ll} = z_1^l z_2^l, \quad \Pi_{l, -l} = 1, \quad \Pi_{l0} = \frac{l!}{[(2l)!]^{1/2}} \sum_{k=0}^l (C_l^k)^2 z_1^k z_2^{l-k}; \quad (18)$$

Π_{lm} and $\Pi_{l, -m}$ are related by

$$\Pi_{lm}(z_1, z_2) = (z_1 z_2)^m \Pi_{l, -m}(z_1, z_2). \quad (19)$$

Compared with the usual formulas for the wave functions of the hydrogen atom in the x or p representation, the expressions (14) and (15) have a very simple form. The scalar product is given by

$$(f, g) = \frac{n^2}{\pi^2} \int \frac{dz_1 dz_2}{[1 + |z_1|^2][1 + |z_2|^2]^{n+1}} f^*(z_1, z_2) g(z_1, z_2), \quad (20)$$

which contains n explicitly. This explains the circumstance that the states $|nlm\rangle$ and $|n'l'm'\rangle$ for $n \neq n'$

can be represented by one and the same function. For example,

$$|n, l, -l\rangle = A_{nl}(z_1 - z_2)^{n-l-1}. \quad (21)$$

In particular, for $l = l_{\max} = n - 1$, $|n, l, -l\rangle = 1$ for all n . Of particularly simple form are the wave functions for s states:

$$|n00\rangle = \frac{1}{\sqrt{n}} (z_1 - z_2)^{n-1}. \quad (22)$$

Expanding $\psi_{nlm}(z_1, z_2)$ in terms of the functions (14), we obtain

$$|nlm\rangle = \sum_{\mu_1 + \mu_2 = m} C_{j\mu_1; j\mu_2}^{lm} |n_1 n_2 m\rangle, \quad (23)$$

where $j = (n - 1)/2$, μ_1 and μ_2 are defined by (6), and $C_{j\mu_1; j\mu_2}^{lm}$ is a Clebsch-Gordan coefficient [for which an expression in the Van der Waerden form is obtained from (15) [14]]. Once this formula is established in the z representation, it remains true in any other representation. One must, however, make sure that the functions $|n_1 n_2 m\rangle$ form a canonical basis [i.e., that the relations (13) are fulfilled]. To this end one may be forced to introduce phase factors. Thus, in the x representation,¹⁾

$$\begin{aligned} |n_1 n_2 m\rangle &= (-)^{n_1 + (m - |m|)/2} \psi_{n_1 n_2 m}(\xi, \eta, \varphi), \\ |nlm\rangle &= (-)^l \psi_{nlm}(\mathbf{r}) = (-)^l R_{nl}(\mathbf{r}) Y_{lm}(\mathbf{n}), \end{aligned} \quad (24)$$

where the functions $\psi_{n_1 n_2 m}(\xi, \eta, \varphi)$ and $R_{nl}(\mathbf{r})$ are defined in [12].

2. CONNECTION BETWEEN THE COULOMB SCATTERING PHASE AND THE CLEBSCH-GORDAN COEFFICIENT

When we go to the region $E > 0$, we encounter the cut $0 < E < \infty$, on whose upper edge

$$n = \frac{1}{\sqrt{-2E}} = \frac{i}{k}. \quad (25)$$

In x space this choice of sign corresponds to an outgoing wave. Introducing the hermitian operator N , we have

$$\begin{aligned} N = -iM &= (2H)^{-1/2} A, \quad J_{1,2} = \frac{1}{2}(L \pm iN), \\ J_1^2 = J_2^2 &= -1/4(1 + 1/k^2) = j(j + 1), \end{aligned} \quad (26)$$

where

$$j = \frac{n-1}{2} = \frac{1}{2} \left(-1 + \frac{i}{k} \right). \quad (27)$$

Setting $m = 0$ in (23) and using (24), we find

$$\psi_{n_1 n_2 0}(\xi, \eta) = (-)^{n_1} \sum_{l=0}^{n-1} C_{j-\mu_1, j\mu_2}^{l0} \psi_{nl0}(\mathbf{r}), \quad (28)$$

where $\mu_1 = (n_1 - n_2)/2$. We obtain the analog of this expansion for the continuous spectrum; in this way we shall find the Clebsch-Gordan coefficients for the generalized "representations" of the group $SU(2)$

¹⁾ We note that the expansion (23) was first obtained by Park; [15] however, the phase factors entering in (24) were not taken into account by him. A formula which is practically equivalent to (23) for the wave functions in p space is contained in the work of Stone [16] (cf. also [6]). This formula has proved convenient for the parametrization of the relativistic scattering amplitude for particles with spin. [17]

corresponding to complex values (27) of the angular momentum.

Let us consider the function $\psi_{\mathbf{k}}^+$ for an attractive Coulomb field:^[12]

$$\psi_{\mathbf{k}}^+ = (2\pi)^{-3/2} e^{i\pi/2} \Gamma(1 - i/k) f_1(\xi) f_2(\eta), \quad (29)$$

where

$$\begin{aligned} \xi &= r + z, & \eta &= r - z, \\ f_1(\xi) &= e^{i k \xi^2/2}, & f_2(\eta) &= e^{-i k \eta^2/2} F(i/k, 1, i k \eta). \end{aligned} \quad (30)$$

In (29), the momentum \mathbf{k} of the incident particles is directed along the z axis, so that $m = 0$, $n_i = -\frac{1}{2} + n\beta_i$ ($i = 1, 2$; β_i are separation constants). The constant β_1 enters in the equation for $f_1(\xi)$:

$$\frac{d}{d\xi} \left(\xi \frac{df_1}{d\xi} \right) + \left(\frac{k^2}{4} \xi + \beta_1 \right) f_1 = 0 \quad (31)$$

[an analogous equation holds for $f_2(\eta)$]. Then

$$\begin{aligned} \beta_1 &= -\frac{ik}{2}, & \beta_2 &= 1 + \frac{ik}{2}, & n_1 &= 0, & n_2 &= \frac{i}{k} - 1 = 2j, \\ \mu_1 &= -\mu_2 = -j. \end{aligned} \quad (32)$$

Using these equalities, we find for the expansion (28)

$$\tilde{\Psi}_{0n,0}(\xi, \eta) = \sum_l C_{jj; j-j}^{l0} \tilde{\Psi}_{nl0}(\mathbf{r}), \quad (33)$$

where $\tilde{\Psi}_{n_1 n_2 0}$ and $\tilde{\Psi}_{nlm}$ are the analytic continuations of the corresponding functions of the discrete spectrum on the upper rim of the cut $0 < E < \infty$.

Using the explicit expressions^[12] for the functions $\tilde{\Psi}_{n_1 n_2 m}(\xi, \eta, \varphi)$ and $\tilde{\Psi}_{nlm}(\mathbf{r})$, we find

$$A = -2k^{1/2} e^{-i\delta_1} [\pi(1 - e^{-2\pi/k})]^{1/2}, \quad B = -k [i(1 - e^{-2\pi/k})]^{1/2}. \quad (34)$$

On the other hand, we have

$$\psi_{\mathbf{k}}^+ = \sum_{l=0}^{\infty} i^l \left(\frac{2l+1}{4\pi} \right)^{1/2} \frac{e^{i\delta_l}}{k} \Psi_{kl0}(\mathbf{r}). \quad (35)$$

Comparison of (33) to (35) yields

$$C_{jj; j-j}^{l0} = i^l \left(\frac{2l+1}{4\pi} \right)^{1/2} \frac{e^{i\delta_l} A}{k B} = [-ik(2l+1)]^{1/2} i^l e^{i(\delta_l - \delta)}, \quad (36)$$

where δ_l is the Coulomb scattering phase:

$$\delta_l = \arg \Gamma(l+1 - i/k) = \arg \Gamma(l - 2j).$$

Let us now make more precise to which representations of the group $SU(2)$ the calculated Clebsch-Gordan coefficient refers. As is known, the usual (finite-dimensional) representations are characterized by a single number, the weight j ($j = 0, \frac{1}{2}, 1, \dots$). The problem of the generalization of the concept of a representation to complex values of j was posed by the development of reggeism and has been considered in many papers.^[18-22] As shown in^[19], a new invariant μ appears in going over to the complex plane, so that the generalized "representation" of the group $SU(2)$ is given by the pair of numbers (j, μ). These numbers determine the spectrum of the operators \mathcal{J}^2 and J_z :

$$\mathcal{J}^2 \psi_{jm} = j(j+1) \psi_{jm}; \quad J_z \psi_{jm} = (\mu + s) \psi_{jm}, \quad (37)$$

where $s = 0, \pm 1, \pm 2, \dots$. For the usual representations $\mu = j - [j]$ and is thus not independent of j (here $[x]$ is the integer part of the number x). As is seen from (32), the representations realized on the hydrogen functions do not belong to the most general type either. In

these representations there exists the vector ψ_{jm} with $m = -j$ or $m = j$. In the first case, setting $m = -j + n$, $\psi_{jm} \equiv f_{jn}$, we have from (13)

$$J_+ f_{jn} = [(n+1)(2j-n)]^{1/2} f_{j, n+1}, \quad J_- f_{jn} = [n(2j+1-n)]^{1/2} f_{j, n-1}, \quad J_0 f_{jn} = (n-j) f_{jn}, \quad (38)$$

i.e., the set of vectors f_{jn} with $n = 0, 1, 2, \dots$ forms an invariant space. Although this representation is infinite-dimensional, there exists a lowest vector f_{j0} for which $J_- f_{j0} = 0$. We shall denote this representation by $D_j^{(+)}$. Analogously, in the second case the vectors ψ_{jm} with $m = j - n$ ($n = 0, 1, 2, \dots$) form an invariant space having a highest vector with $n = 0$. This representation is denoted by $D_j^{(-)}$.

The representations $D_j^{(+)}$ and $D_j^{(-)}$ are, as it were, in the transition region between the degenerate case of finite-dimensional representations (when the spectrum of the operator J_z is bounded from below and above) and the general case²⁾, as has been pointed out in^[19]. Subsequently these representations have been studied in detail by Sannikov.^[22]

The wave functions of the hydrogen atom in parabolic coordinates form the representation $D_j^{(+)} \otimes D_j^{(-)}$, where j lies on the straight line $\text{Re } j = -\frac{1}{2}$ [cf. (27)]. The transition from parabolic to spherical coordinates corresponds to the expansion of this representation into irreducible ones. It is interesting to note that this expansion involves only the usual values of the angular momentum $l = 0, 1, 2, \dots$.

The Clebsch-Gordan coefficient $C_{jj; j-j}^{l0}$ for the usual values of j has the form (cf. [14])

$$C_{jj; j-j}^{l0} = \left\{ (2l+1) \frac{[(2j)!]^2}{(2j+1+l)!(2j-l)!} \right\}^{1/2}. \quad (39)$$

Changing the factorials to Γ functions and substituting formally the value j from (27), we arrive at (36). Thus in the given special case, the value of the Clebsch-Gordan coefficient for complex j agrees with its analytic continuation from integer and half-integer values of the angular momentum.

The example considered shows that the problem of the coupling of complex angular momenta is practically already encountered in ordinary quantum mechanics (at least for some values of j). This confirms the possibility of a group-theoretical interpretation of the complex angular momentum. Thus a number of problems whose mathematical solution meets with difficulties, can be considered on the example of the hydrogen atom.³⁾

²⁾ As is seen from (38), the representations $D_j^{(+)}$ and $D_j^{(-)}$ are, strictly speaking, irreducible representations of the Lie algebra. The problem of their extension to representations of the rotation group as a whole is not trivial and requires a separate investigation.

³⁾ For example, the problem of the expansion of the direct product of two "representations" of the group $SU(2)$ corresponding to arbitrary complex values j_1 and j_2 has not yet been solved in general form. It is therefore impossible to tell whether the Clebsch-Gordan coefficient for complex j is the analytic continuation of the usual coefficients, as is frequently assumed. The answer obtained above for the special case $j_1 = j_2 = (-1 + i/k)/2$ is of interest in the sense that it shows that the usual values (integer or half-integer) may appear in the coupling of two complex angular momenta. It may be that there is a connection with the problem of constructing the usual particles from the unobserved "quarks" with complex spins (this remark is due to I. S. Shapiro).

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