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The harmonic oscillator: values of the SU(3) invariants

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Abstract. Formulae are given relating the Hamiltonian of the three-dimensional harmonic oscillator to the second and third order invariants I_2 and I_3 , respectively, of its symmetry group SU(3). For those irreducible representations which are realized by wavefunctions of the harmonic oscillator, I_2 and I_3 are diagonal operators satisfying the relationship $6I_3 = I_2(4I_2 + 1)^{1/2}$.

1. Introduction

It is well known that the n -dimensional harmonic oscillator possesses the unimodular unitary group in n dimensions, SU(n), as a symmetry group, that is, SU(n), whose generators can be expressed as operators commuting with the harmonic oscillator Hamiltonian, completely accounts for the system's energy degeneracy. This was shown for the two-dimensional case by Jauch and Hill (1940) and the generalization to the n -dimensional case discussed by Allen Baker Jr (1956). A discussion of the three-dimensional case is given by Lipkin (1965) and by Elliott (1958a, b, 1963), and Bargmann and Moshinsky (1960, 1961) in which the decomposition of the irreducible representations of SU(3) on restriction to its rotation subgroup O(3) is treated in great detail.

In the treatments of the three-dimensional harmonic oscillator given so far, the irreducible representations of SU(3) are described in terms of Young tableaux (or, equivalently, in terms of highest weights), it being shown that the energy levels correspond to a restricted class of representations, determined by the requirement of symmetry under permutations of the oscillator quanta (Lipkin 1965). The alternative specification of the irreducible representations in terms of the values of the group invariants is not used, although Bisiacchi and Budini (1966), by working backwards from the expression for the energy levels, do deduce what values these invariants must have. This treatment contrasts sharply with the usual group theoretical treatment of the hydrogen atom as summarized by, for instance, Bander and Itzykson (1966) and Hughes (1967), in which expressions for the invariants of the symmetry group in terms of the Hamiltonian are used to determine the energy levels and the irreducible representations which correspond to them.

The purpose of this paper is to give a parallel treatment of the three-dimensional harmonic oscillator, in which expressions are obtained giving the second and third order invariants I_2 and I_3 , respectively, in terms of the Hamiltonian H , and these used to derive the energy levels and the corresponding irreducible representations of SU(3). We shall find that those occurring are the ones for which the values of the invariants satisfy the nonlinear relationship

$$6I_3 = I_2(4I_2 + 1)^{1/2}.$$

Although no significantly new light is shed on the properties of the harmonic oscillator by this treatment, the relationship between I_2 and I_3 is interesting because of its non-linear nature. More specifically, it shows that those irreducible representations of the symmetry group of a quantum mechanical system which are realized by the states of the system need not be the ones for which all but one of the invariants vanish (Budini 1966).

2. The SU(3) symmetry group

The Schrödinger equation for the three-dimensional harmonic oscillator is

$$H\psi(\mathbf{r}) = E\psi(\mathbf{r}) \quad (1)$$

where the Hamiltonian H is given by

$$H = -\frac{1}{2\mu} \left(\frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} + \frac{\partial^2}{\partial x_3^2} \right) + \frac{k}{2} (x_1^2 + x_2^2 + x_3^2). \quad (2)$$

μ is the mass of the oscillator, $\mathbf{r} \equiv (x_1, x_2, x_3)$ its position vector relative to the centre of the potential, and k a positive constant giving the strength of the potential. A system of units in which $\hbar = 1$ is employed. We shall find it notationally convenient to use a set of coordinates $\mathbf{r}' \equiv (x'_1, x'_2, x'_3)$ defined by

$$\mathbf{r}' = (\mu k)^{1/4} \mathbf{r}, \quad (3)$$

and the normalized 'Hamiltonian'

$$H' = -(\mu/k)^{1/2} H. \quad (4)$$

H' is given in terms of the new coordinates by the formula

$$H' = \frac{1}{2} \left\{ \left(\frac{\partial^2}{\partial x'^2_1} + \frac{\partial^2}{\partial x'^2_2} + \frac{\partial^2}{\partial x'^2_3} \right) - (x'^2_1 + x'^2_2 + x'^2_3) \right\}. \quad (5)$$

From the obvious rotational symmetry of the system, which is intimately related to the separability of its Schrödinger equation in spherical polar coordinates, it follows that the three-dimensional rotation group O(3), generated by the angular momentum operators

$$L_1 = -i \left(x'_2 \frac{\partial}{\partial x'_3} - x'_3 \frac{\partial}{\partial x'_2} \right),$$

etc, is a symmetry group, and this immediately explains the degeneracy of its energy levels with respect to the magnetic quantum number m . However, the harmonic oscillator shares with the hydrogen atom the property that its energy levels are also degenerate in the total angular momentum quantum number l ; this extra degeneracy cannot be accounted for by O(3) symmetry alone and is a consequence of the possession by both systems of a larger symmetry group, O(4) for the hydrogen atom and SU(3) for the harmonic oscillator.

The extra symmetry of the harmonic oscillator is related to the fact that (again, as in the case of the hydrogen atom) its Schrödinger equation can be separated in other coordinate systems as well as in spherical polars. From the extra constants of separation that arise one obtains new operators commuting with the Hamiltonian and, by repeated commutation of these amongst themselves and with the angular momentum operators until closure is achieved, one obtains the generators of the larger symmetry group.

Using separability of the harmonic oscillator's Schrödinger equation in either rectangular or cylindrical polar coordinates and carrying out the above procedure one arrives at the following set of nine hermitian operators which commute with H' :

$$L_i = -i \left(x'_j \frac{\partial}{\partial x'_k} - x'_k \frac{\partial}{\partial x'_j} \right), \tag{6}$$

$$M_i = \frac{\partial^2}{\partial x'_j \partial x'_k} - x'_j x'_k, \tag{7}$$

$$N_i = \frac{1}{2} \left(\frac{\partial^2}{\partial x_i'^2} - x_i'^2 \right), \tag{8}$$

where in (6) and (7), (i, j, k) are cyclic permutations of $(1, 2, 3)$ and in (8) $i = 1, 2, 3$.

These operators satisfy the following commutation relations:

$$[L_1, L_2] = -[M_1, M_2] = [M_3, N_2] = -[M_3, N_1] = iL_3$$

and two similar equations obtained from these by cyclic permutations

$$[L_1, M_2] = -[L_2, M_1] = [L_3, N_2] = -[L_3, N_1] = -iM_3$$

and cyclic permutations

$$[L_1, M_1] = 2i(N_3 - N_2)$$

and cyclic permutations,

$$[N_i, N_j] = [N_i, M_i] = [N_i, L_i] = 0, \quad i = 1, 2, 3. \tag{9}$$

The N also satisfy the relationship

$$N_1 + N_2 + N_3 = H'. \tag{10}$$

The nine operators together generate the group U(3), isomorphic to the direct product of SU(3) and U(1), the latter group being generated by H' . However, no useful purpose is achieved by including the Hamiltonian of a system amongst the generators of its symmetry group, so the above set of nine operators must be replaced by an independent set of eight operators from which the Hamiltonian is excluded.

A convenient choice for these eight operators is given by

$$\begin{aligned} H_1 &= (2\sqrt{3})^{-1} L_3, & H_2 &= 6^{-1} (2N_3 - N_1 - N_2) \\ E_{\pm\alpha} &= -(2\sqrt{6})^{-1} (N_1 - N_2 \pm iM_3) \\ E_{\pm\beta} &= -(4\sqrt{3})^{-1} (L_1 \pm iL_2 + M_2 \pm iM_1) \\ E_{\pm\bar{\beta}} &= (4\sqrt{3})^{-1} (L_1 \pm iL_2 - M_2 \mp iM_1). \end{aligned} \tag{11}$$

H_1 and H_2 are hermitian operators, whereas $E_{+\alpha}$ and $E_{-\alpha}$ are hermitian conjugates as are, respectively, $E_{+\beta}$ and $E_{-\beta}$, and $E_{+\bar{\beta}}$ and $E_{-\bar{\beta}}$. These operators are precisely the generators of SU(3) as given by Baird and Biedenharn (1963), where their commutation relations can be found.

We end this section by noting one major difference in the way in which the symmetry groups arise for the harmonic oscillator and hydrogen atom. In the latter case (Bander and Itzykson 1966), the commutation relations of the operators commuting with the Hamiltonian involve the Hamiltonian itself. Consequently the energy has to be given a fixed value E , say, and the operators renormalized by a factor involving E before they

can be used to generate the symmetry group. According as E is fixed at a negative or positive value, one obtains the group $O(4)$ or the noncompact group $O(3, 1)$. In the case of the harmonic oscillator the Hamiltonian does not appear in the commutation relations, and the single group $SU(3)$ is generated immediately without either any restriction to a fixed energy value or any renormalization being necessary.

3. Relationship between the invariants

Now that we have shown that $SU(3)$ is the symmetry group of the harmonic oscillator, we determine which of its irreducible representations are realized by the system, and in so doing also derive the well known formula for the energy levels. $SU(3)$ possesses two invariants I_2 and I_3 , whose forms in terms of the generators (11) have been given by Baird and Biedenharn (1963) and are

$$I_2 = H_1^2 + H_2^2 + E_\alpha E_{-\alpha} + E_{-\alpha} E_\alpha + E_\beta E_{-\beta} + E_{-\beta} E_\beta + E_{\bar{\beta}} E_{-\bar{\beta}} + E_{-\bar{\beta}} E_{\bar{\beta}}, \tag{12}$$

$$I_3 = \frac{1}{6}H_2(H_2^2 - 1) - \frac{1}{2}H_2 I_2 + \frac{1}{2}(H_1^2 + E_\alpha E_{-\alpha} + E_{-\alpha} E_\alpha)(3H_2 - 1) + \sqrt{3}H_1(E_\beta E_{-\beta} - E_{-\beta} E_\beta) + \sqrt{6}(E_{-\alpha} E_\beta E_{\bar{\beta}} + E_\alpha E_{-\bar{\beta}} E_{-\beta}). \tag{13}$$

These commute with all the group generators, and therefore their eigenvalues serve as a unique label for the irreducible representations. Defining p and q by the equations

$$I_2 = \frac{1}{9}(p^2 + q^2 - pq + 3p) \tag{14}$$

and

$$I_3 = \frac{1}{162}(p - 2q)(2p + 3 - q)(p + q + 3), \tag{15}$$

Baird and Biedenharn show that every unitary irreducible representation of $SU(3)$ is specified by the pair of integers (p, q) satisfying $p \geq q \geq 0$, the dimension of the representation (p, q) being $\frac{1}{2}(p - q + 1)(p + 2)(q + 1)$. Furthermore, the representations (p, q) and $(p, p - q)$ are mutually contragredient, from which we see that contragredient representations correspond to the same value of I_2 , and to opposite signs of the values of I_3 .

By the substitution of equations (11) in (12) and (13) we obtain expressions for I_2 and I_3 in terms of the operators L_i, M_i and N_i ($i = 1, 2, 3$); by the further use of equations (6), (7) and (8) I_2 and I_3 can be expressed as differential operators in x'_1, x'_2 and x'_3 . Finally, employing equation (5) for H' , we find that I_2 and I_3 are given in terms of H' by the formulae

$$I_2 = \frac{1}{9}(H'^2 - \frac{9}{4}) \tag{16}$$

and

$$I_3 = -\frac{1}{81}(H'^2 - \frac{9}{4})H'. \tag{17}$$

From equation (16) we obtain $H' = \pm \frac{3}{2}(4I_2 + 1)^{1/2}$; to decide which sign to take we must consider the definition of the Hamiltonian in terms of the momentum operators $p_i = -i(\partial/\partial x_i)$; this is

$$H = \frac{1}{2\mu}(p_1^2 + p_2^2 + p_3^2) + \frac{k}{2}(x_1^2 + x_2^2 + x_3^2)$$

and so, since both μ and k are positive constants, H is a positive definite operator with

positive eigenvalues. H' , therefore, has negative eigenvalues, so the relationship between H' and I_2 must be

$$H' = -\frac{3}{2}(4I_2 + 1)^{1/2}. \quad (18)$$

Substitution of this into (17) yields the nonlinear relationship

$$I_3 = +\frac{1}{6}I_2(4I_2 + 1)^{1/2}. \quad (19)$$

This is the condition which must be satisfied by the eigenvalues of the invariants in order that the corresponding representations of $SU(3)$ be realized by the harmonic oscillator wavefunctions. To obtain their specification in terms of (p, q) we square (19) and use (14) and (15) for I_2 and I_3 . After a short calculation this yields the equation

$$0 = 36I_3^2 - I_2^2(4I_2 + 1) = -\frac{1}{27}q(p-q)(p+1)(p+3)(q+2)(p-q+2). \quad (20)$$

The only solution of this equation consistent with the conditions that p, q be integers satisfying $p \geq q \geq 0$ are clearly $q = 0$ or $q = p$, so the possible representations are the $(p, 0)$ or the contragredient (p, p) . However, I_3 is negative for the latter case, whereas to be applicable to the harmonic oscillator it must be positive, so we finally obtain the appropriate representations to be the $(p, 0)$, where $p = 0, 1, 2, \dots$. The corresponding values of the invariants are $I_2 = \frac{1}{9}p(p+3)$ and $I_3 = \frac{1}{162}p(p+3)(2p+3)$, from which one easily obtains the eigenvalues $-(p+\frac{3}{2})$ for H' . Finally, using $H' = -(\mu/k)^{1/2}H$, we deduce that the energy levels of the harmonic oscillator are E_p , where

$$E_p = \left(\frac{k}{\mu}\right)^{1/2} \left(p + \frac{3}{2}\right), \quad p = 0, 1, 2, \dots \quad (21)$$

The degeneracy of the level E_p equals the dimensions of the representation $(p, 0)$ and is therefore $\frac{1}{2}(p+1)(p+2)$.

Thus, by means of a group theoretical treatment which precisely parallels that used for the hydrogen atom, we have rederived the well known formulae for the harmonic oscillator energy levels and their degeneracies.

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