

Group Xheoretic Derivation of Angular Functions for the Non-Relativistic A-Body Problem in the K-Harmonics Approach

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A derivation of an angular basis for the A-body problem, suitable for the K-harmonics method, is presented. Those angular functions are obtained from homogeneous and harmonic polynomials, which are completely specified by labels associated to eigenvalues of the Casimir invariants of subgroups of the $3(A-1)$ -dimensional orthogonal group, among them, the total angular momentum and its z-projection.

Constrói-se uma base angular, para o problema a A corpos, adequada para o método dos K-harmônicos. Essas funções são obtidas de polinômios homogêneos e harmônicos, completamente rotulados por números associados a autovalores de operadores de Casimir de subgrupos do grupo ortogonai em $3(A-1)$ dimensões. Entre esses números, destacam-se o momento angular total e sua 3.^a componente.

1. Introduction

A method for obtaining the binding energy and wave function of a system of A particles, the K-harmonics method, was introduced by Zickendraht¹ and Simonov². The starting point of the method is to expand the wave function of the system in terms of a complete set of angular functions (the K-harmonics) over the unit sphere of the $3(A-1)$ -dimensional vector space of relative coordinates of the A particles. The construction of the K-harmonics is, therefore, essential to the method.

Methods for constructing the K-harmonics, for $A = 3$ and 4, are found in the literature. In a recent paper, Louck and Galbraith³ review these methods and present some new results in the framework of applications of orthogonal and unitary group techniques to the A-body problem. They present (their Section VII) a set of harmonic and homogeneous polynomials that could be useful in the K-harmonics method. However, these polynomials present, as they have mentioned, some difficulties, namely: a) there are some labels which have no group theoretic

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meaning; b) the polynomials are not, in general, orthogonal in these labels; c) they have no permutational symmetry.

In this paper, we present a basis of homogeneous and harmonic polynomials with definite total angular momentum and z-projection that we hope can be useful to the *K*-harmonics method. The way in which they are constructed is a generalization of the method of Ref. 4, hereby referred to as I, for the case $A = 3$. The results are close to those of Louck and Galbraith, but we have solved the difficulties a) and b), mentioned above. The permutational symmetry is, however, an open problem. Even in the case $A = 3$, it is a difficult task, as can be seen in I. The case $A = 4$, can be solved (see Ref. 5) exploiting a property of the $S(4)$ group which have no analog for the, general, $S(n)$, namely $S(4)$ is the semidirect product of the four-group $D(2)$ by $S(3)$, which allows to give the solution for $A = 4$ in terms of the one for $A = 3$.

Most of the formulas of this paper are not new (see, e.g., Ref. 6). The new feature of our paper is, besides given an explicit derivation of the *K*-harmonics, to show, explicitly, the group-theoretic aspects involved in the problem (which are not transparent in the *K*-harmonics literature) improving, in this way, the understanding of those formulas.

In Section 2, we show how the group $O_{3(A-1)}$ is related to the *A*-body problem. In Section 3, the basis is explicitly constructed, while, in Section 4, the chain of the $O_{3(A-1)}$ subgroups involved is discussed. Finally, in Section 5, hyperspherical coordinates are introduced.

2. The Orthogonal Group $O_{3(A-1)}$

In the center of mass frame, the non-relativistic kinetic energy operator, for a system of *A* particles with equal masses reads

$$H = -\frac{1}{2} \sum_{i=1}^{A-1} \nabla_{\mathbf{x}^i}, \quad (\hbar = m = 1), \quad (2-1)$$

where the \mathbf{x}^i 's are Jacobi coordinates of the relative motion. These coordinates are defined by

$$\mathbf{x}^i = \frac{1}{\sqrt{i(i+1)}} \left[\sum_{j=1}^i \mathbf{r}^j - i \mathbf{r}^{i+1} \right], \quad i = 1, 2, \dots, (A-1), \quad (2-2)$$

where $\mathbf{r}^i (i=1, 2, \dots, A)$ is the position vector of particle i , relative to the laboratory frame of reference. Together with

$$\mathbf{X}^A = \frac{1}{\sqrt{A}} \sum_{i=1}^A \mathbf{r}^i, \quad (2-3)$$

they are related to the \mathbf{x}^i 's by a real orthogonal transformation.

The components of \mathbf{x}^i may be put in a one-to-one correspondence with a $3(A-1)$ -dimensional vector \mathbf{v} by, say,

$$v_{3(i-1)+j} = (\mathbf{x}^i)_j, \quad i = 1, 2, \dots, A-1, \quad (2-4)$$

$$j = 1, 2, 3.$$

In this way, the RHS of (2-1) becomes proportional to the Laplacian operator in $3(A-1)$ dimensions and it is well known that this operator is invariant under the group of orthogonal transformations, whose generators are here realized by

$$\Lambda_{ij}^{\alpha\beta} = \frac{1}{2} \left(x_i^\alpha \frac{\partial}{\partial x_j^\beta} - x_j^\beta \frac{\partial}{\partial x_i^\alpha} \right), \quad \alpha, \beta = 1, 2, \dots, (A-1), \quad (2-5)$$

$$i, j = 1, 2, 3,$$

where x_i^α is the i -component of \mathbf{x}^a . It is easy to verify that these generators satisfy the usual commutation relations of the generators of orthogonal groups, namely,

$$[\Lambda_{ij}^{\alpha\beta}, \Lambda_{kl}^{\gamma\delta}] = \frac{1}{2} (\Lambda_{il}^{\alpha\gamma} \delta^{\beta\mu} \delta_{jk} - \Lambda_{ik}^{\alpha\mu} \delta^{\beta\gamma} \delta_{jl} + \Lambda_{jk}^{\beta\mu} \delta^{\alpha\gamma} \delta_{il} - \Lambda_{jl}^{\beta\gamma} \delta^{\alpha\mu} \delta_{ik}). \quad (2-6)$$

It is clear from (2-5) that the generators of $O_{3(A-1)}$ maintain the degree of homogeneous polynomials in the variables v_i and it follows, therefore, that the set of homogeneous polynomials of a given degree λ , in the variables $v_i (i=1, 2, \dots, 3(A-1))$, carry a representation of $O_{3(A-1)}$. Such a representation is, in general, reducible, as we shall see in Section 3. Irreducible representations (hereby denoted as irrep) are obtained by requiring that the homogeneous polynomials be harmonic in the $3(A-1)$ variables.

The Casimir invariant of $O_{3(A-1)}$, namely,

$$\mathcal{I}_2 = \frac{1}{2} \sum_{i,j,\alpha,\beta} \Lambda_{ij}^{\alpha\beta} \Lambda_{ji}^{\beta\alpha}, \quad (2-7)$$

assumes, with the realization (2-5) of the generators, the form

$$\mathcal{J}_2 = -v^2 \nabla^2 + (\mathbf{v} \cdot \nabla)^2 + (3A-5)\mathbf{v} \cdot \nabla. \quad (2-8)$$

Therefore, in the space of homogeneous and harmonic polynomials, of degree λ , in v_i , it is diagonal with eigenvalue $\lambda(\lambda + 3A - 5)$. The higher order invariants, either vanish identically or can be written as functions of V^2 and the Euler operator $\mathbf{v} \cdot \nabla$. Thus, the label λ is enough to characterize the irreducible representation of $O_{3(A-1)}$ carried by the homogeneous and harmonic polynomials of degree λ . This representation is, indeed, the so-called "most degenerate representation" of $O_{3(A-1)}$, characterized by Gel'fand labels $[A, 0, \dots, 0]$ to which we will refer as $[\lambda]$.

3. Construction of the Basis

In this section, a basis for the irrep $[\lambda]$ of $O_{3(A-1)}$, associated to the A-particle system, will be constructed by induction, starting from the basis for the O_6 group, associated to a system of 3 particles. In this way, we assume that we already have a basis for $O_{3(A-2)}$, associated to a $(A-1)$ -particle system and, then, relate the basis of $O_{3(A-1)}$ to it. The feasibility of this procedure lies in the fact that when we go from the Jacobi relative vectors, for $A-1$ particles, to those for A particles, the previous vectors remain unchanged and all we have to do is simply add one extra Jacobi vector (which is the only one to depend on the position vector of the A^{th} particle).

Let

$$P_{(\alpha)_{A-1} L_{A-1} M_{A-1}}^{[\lambda_{A-1}]}(\mathbf{x}^1, \mathbf{x}^2, \dots, \mathbf{x}^{A-2}) \quad (3-1)$$

be the components of the polynomial basis for the $(A-1)$ -particle system. [The subscript $A-1$ in the labels is to make clear that they refer to a $(A-1)$ -particle system.] They carry an irrep of $O_{3(A-2)}$, characterized by the Gel'fand label λ_{A-1} , and have definite total angular momentum L_{A-1} , z-projection M_{A-1} , and a set of labels which we designate, for the moment, by $(\alpha)_{A-1}$ and whose structure will become clear as the process is developed.

In analogy to what was done in I, we make the following Ansatz for the components of the $O_{3(A-1)}$ polynomial bases for the A-particle system:

$$P_{(\alpha)_A L_A M_A}^{[\lambda_A]} = \mathcal{N}_A G_A(\mathbf{x}^1, \dots, \mathbf{x}^{A-1}) \sum_{M_{A-1} l_{A-1} m_{A-1}} \langle L_{A-1} M_{A-1} l_{A-1} m_{A-1} | L_A M_A \rangle \times \\ \times P_{(\alpha)_{A-1} L_{A-1} M_{A-1}}^{[\lambda_{A-1}]}(\mathbf{x}^1, \dots, \mathbf{x}^{A-2}) \mathcal{Y}_{m_{A-1}}^{l_{A-1}}(\mathbf{x}^{A-1}), \quad (3-2)$$

where \mathcal{N}_A is a normalization constant, G_A a function to be determined and $\mathcal{Y}_m^l(\mathbf{x}) = |\mathbf{x}|^l Y_m^l(\hat{\mathbf{x}})$ is a 3-dimensional solid harmonic. Since we want to preserve the labels λ_{A-1} and l_{A-1} , the function G_A can depend on x^1, \dots, x^{A-1} , only through the invariants of the subgroups $O_{3(A-2)}$ and $O_3(x^{A-1})$ of $O_{3(A-1)}$, whose irreps they label. We, therefore, write

$$G_A(\mathbf{x}^1, \dots, \mathbf{x}^{A-1}) \equiv G_A(\rho_{A-1}^2, x_{A-1}^2), \quad (3-3)$$

with

$$\rho_{A-1}^2 = \sum_{i=1}^{A-2} \mathbf{x}^i \cdot \mathbf{x}^i \text{ and } x_{A-1}^2 = \mathbf{x}^{A-1} \cdot \mathbf{x}^{A-1}. \quad (3-4)$$

Of course, $P_{(\alpha)A L_A M_A}^{[\lambda_A]}$ has well defined values of the total angular momentum L_A and its z-projection, M_A .

Imposing that the RHS of (3-2) be a homogeneous polynomial of degree λ_A , in the variables \mathbf{x}^i , we find that G_A has to be a homogeneous polynomial of degree $n_A = \lambda_A - \lambda_{A-1} - l_{A-1}$ and, taking into account that G_A depends on \mathbf{x}^i through quadratic functions (Eqs. 3.3 and 3.4), we have that n_A is an even non-negative integer. We, then, obtain the branching law

$$\lambda_{A-1} + l_{A-1} = \lambda_A, \lambda_A - 2, \dots, \{1\}. \quad (3-5)$$

On the other hand, the harmonicity of (3-2) and the fact that

$$P_{(\alpha)A-1 L_{A-1} M_{A-1}}^{[\lambda_{A-1}]} \text{ and } \mathcal{Y}_{m_{A-1}}^{l_{A-1}}(\mathbf{x}^{A-1})$$

are harmonic and homogeneous polynomials of degree λ_{A-1} and l_{A-1} , respectively, require that G_A has to satisfy the equation

$$\nabla^2 G_A + 4 \left(\lambda_{A-1} \frac{\partial G_A}{\partial \rho_{A-1}^2} + l_{A-1} \frac{\partial G_A}{\partial x_{A-1}^2} \right) = 0. \quad (3-6)$$

From some of the above considerations, we can write G_A as

$$G_A = \sum_{2(\mu+\nu)=n_A} A_\mu (\rho_{A-1}^2)^\mu (x_{A-1}^2)^\nu. \quad (3-7)$$

Substituting (3-7) into (3-6), we get a two-term recurrence relation, which allows us to determine $A_\mu (\mu = 1, 2, \dots, n_A/2)$ in terms of A_0 . With the appropriate choice of A_0 , we finally obtain

$$G_A(\rho_{A-1}^2, x_{A-1}^2) = \sum_{\mu=0}^{N_A} (-)^{\mu} \binom{\alpha_A + N_A}{N_A - \mu} \binom{\beta_A + N_A}{\mu} (\rho_{A-1}^2)^{\mu} (x_{A-1}^2)^{N_A - \mu} \quad (3-8)$$

with

$$\begin{aligned} N_A &= \frac{1}{2} n_A = \frac{1}{2} (\lambda_A - \lambda_{A-1} - l_{A-1}), \\ \alpha_A &= \lambda_{A-1} + \frac{3}{2} A - 4, \\ \beta_A &= l_{A-1} + \frac{1}{2}. \end{aligned} \quad (3-9)$$

Now, the procedure goes down to $A-1, A-2, \dots$, until we get $A=3$, whose solution is given in I (Eqs. 4-3 to 4-5). Going through all these steps, we get

$$\begin{aligned} P_{(\alpha)_A L_A M_A}^{(\lambda_A)} &\equiv \left| \begin{array}{ccccccc} \lambda_A & \lambda_{A-1} & \lambda_{A-2} & \dots & \lambda_5 & \lambda_4 & \lambda_3 \\ l_{A-1} & l_{A-2} & \dots & \dots & l_4 & l_3 & l_2 \\ M_A & L_A & L_{A-1} & L_{A-2} & \dots & L_5 & L_4 & L_3 & L_2 \end{array} \right\rangle = \\ &= \left[\prod_{i=2}^{A-1} \mathcal{N}_{i+1} G_{i+1}(\rho_i^2, x_i^2) \sum_{M_i} \langle L_i M_i l_i m_i | L_{i+1} M_{i+1} \rangle \mathcal{Y}_{m_i}^{l_i}(\mathbf{x}^i) \right] \mathcal{Y}_{M_2}^{L_2}(\mathbf{x}^1). \end{aligned} \quad (3-10)$$

In (3-10), the structure of the multiple label $(\alpha)_A$ is explicitly exhibited. [Since the polynomials (3-10) are homogeneous of degree λ_A , angular functions are obtained just dividing (3-10) by ρ^{λ_A} .] The branching laws, which restrict the different labels, are

$$L_{i+1} = L_i + l_i, L_i + l_i - 1, \dots, |L_i - l_i|, \quad (i=1, 2, \dots, A-1), \quad (3-11)$$

$$\lambda_{i-1} + l_{i-1} = \lambda_i, \lambda_i - 2, \dots, \{1^0, \quad (i=4, 5, \dots, A), \quad (3-12)$$

$$L_2 + l_2 = \lambda_3, \lambda_3 - 2, \dots, \{1^0, \quad (3-13)$$

$$M_A = L_A, L_A - 1, \dots, -L_A.$$

As an immediate consequence of (3-11)-(3-13), we have

$$L_i \leq l_i, \quad i=3, 4, \dots, A. \quad (3-15)$$

We **tried** to encode the branching laws (3-11)-(3-13) and (3-15) by conveniently positioning the labels λ_i, l_i, L_i , in the ket of Eq. (3-10), in analogy to what was done by Gelfand and Zetlin for the unitary groups. Let us explain it.

In the ket (3-10), each $l_i (i = 3, \dots, A - 1)$ is related to its neighbouring λ 's by Eq. (3-12), so each λ_i is equal or greater than its right positioned A and 1 neighbours, as well as equal or greater than their sum. Also, each $l_i (i = 2, \dots, A - 1)$ is related to its L neighbours by the triangular relation (3-11). Finally, each A is greater than or equal to any label below it and at its right.

For the $A = 3$ case, the dimension of the irrep $[\lambda_3]$ is equal to the difference between the number of linearly independent homogeneous polynomials of degree λ_3 , in six variables, minus this number for $\lambda_3 - 2$. We should, then, expect an analogous formula to hold for general A , i.e., that the dimension of the irrep λ_A be given by

$$\begin{aligned} \dim [\lambda_A] &= \binom{\lambda_A + 3A - 4}{\lambda_A} - \binom{\lambda_A + 3A - 6}{\lambda_A - 2} = \\ &= \frac{(2\lambda_A + 3A - 5)}{(3A - 5)} \binom{\lambda_A + 3A - 6}{\lambda_A} \end{aligned} \quad (3-16)$$

This is, indeed, true and can be proved by induction using the branching laws (3-11) to (3-14).

From (3-16), we have

$$\binom{\lambda_A + 3A - 4}{\lambda_A} = \sum_{i=0}^{[\lambda_A/2]} \dim [\lambda_A - 2i]. \quad (3-17)$$

Then, by the same reasoning made in I, we have that **any homogeneous polynomial of degree λ , in v_i , $P^\lambda(v_i)$** , can be written as a linear combination of the homogeneous and harmonic polynomials (3-10) of degrees $A - 1 - 2, \dots$, i.e.,

$$P^\lambda(v_i) = \sum_{j, (\alpha)_A, L_A, M_A} C_{j(\alpha)_A L_A M_A}^\lambda (\rho_A^2)^j P_{(\alpha)_A L_A M_A}^{[\lambda - 2j]}(v_i), \quad (3-18)$$

where $\rho_A^2 = \sum_{i=1}^{A-1} \mathbf{x}^i \cdot \mathbf{x}^i$. This shows that the basis of $O_{3(A-1)}$, carried

by the homogeneous polynomials of **degree λ , in v_i** , is reducible. The irreducibility of the basis carried by the *harmonic* polynomials (3-10) can be proved by showing that the **maximum weight polynomial is unique**.

4. The Chain of $O_{3(A-)}$ Subgroups

From Section 3, we see that in each stage of the building up process of construction of the basis (3-10) of $O_{3(A-1)}$, we have the following links in a chain of $O_{3(A-1)}$ subgroups:

$$O_{3(i-1)} \supset [O_{3(i-2)} \otimes O_3(\mathbf{x}^{i-1})] \quad , i = 3, 4, \dots, A, \quad (4-1)$$

$$\cup$$

$$O_3(\mathbf{L}_i)$$

where $O_3(\mathbf{x}^{i-1})$ and $O_3(\mathbf{L}_{i-1})$ are groups of orthogonal transformations in the three-dimensional spaces of vectors \mathbf{x}^{i-1} and of generators \mathbf{L}_{i-1} (total angular momentum of physical system of particles $1, 2, \dots, (i-1)$), respectively. Therefore, the chain of $O_{3(A-1)}$ subgroups, whose labels were used to specify the hyperspherical solid harmonics (3-10), is

$$O_{3(A-1)} \supset [O_{3(A-2)} \otimes O_3(\mathbf{x}^{A-1})] \supset \dots \supset [O_6 \otimes O_3(\mathbf{x}^3)] \supset [O_3(\mathbf{x}^2) \otimes O_3(\mathbf{x}^1)]$$

$$\cup \quad \cup \quad \cup$$

$$O_3(\mathbf{L}_A) \quad \supset \dots \supset \quad O_3(\mathbf{L}_4) \quad \supset \quad O_3(\mathbf{L}_3) \quad (4-2)$$

$$\cup$$

$$O_2(M_A)$$

5. Hyperspherical Coordinates and Normalization

We now introduce a scalar product in the vector space spanned by the polynomials (3-10) in the way which is the usual one in the K-harmonics literature, namely,

$$(P, Q) = \int P^* Q d\Omega_A, \quad (5-1)$$

where $d\Omega_A$ is the surface element in the unit sphere imbedded in a $3(A-1)$ dimensional Euclidian space, and P, Q are any two square-integrable functions of v_i .

To make (5-1) explicit, we need to introduce hyperspherical coordinates. The radial coordinate is given by

$$\rho_A^2 = \sum_{i=1}^{3(A-1)} v_i^2 \equiv \sum_{i=1}^{A-1} \mathbf{x}^i \cdot \mathbf{x}^i. \quad (5-2)$$

For the angular coordinates, we have a good deal of freedom. The most convenient choice is dictated by the building up procedure itself, which we discussed in Section 3. Indeed, since we have

$$\rho_A^2 = \rho_{A-1}^2 + x_{A-1}^2, \quad (5-3)$$

it is then quite natural to write

$$\rho_{A-1}^2 = \rho_A^2 \sin^2 \chi_A, \quad x_{A-1}^2 = \rho_A^2 \cos^2 \chi_A, \quad (5-4)$$

with $0 < \chi_A < \pi/2$.

With this parametrization, the function G_A (Eq. 3-8) becomes

$$G_A(\rho_{A-1}, x_{A-1}^2) = (\rho_A^2)^{n_A} P_{N_A}^{(\alpha_A, \beta_A)}(\cos 2\chi_A) \quad (5-5)$$

where $P_N^{(\alpha, \beta)}(x)$ is a **Jacobi Polynomial**¹⁰, while α , β and N are given by Eqs. (3-9).

From (5-3), it follows an identity linking $d\Omega_A$ to the solid angle element $d\Omega_{A-1}$ for $A-1$ particles, namely,

$$d\Omega_A = \cos^2 \chi_A (\sin^2 \chi_A)^{3A-7} d\chi_A d\Omega(\mathbf{x}^{A-1}) d\Omega_{A-1}, \quad (5-6)$$

where $d\Omega(\mathbf{x}^{A-1})$ is the usual solid angle element in the three-dimensional space of vectors \mathbf{x}^{A-1} .

Making use of (5-6), it is a simple matter to show that the polynomials (3-2) are orthogonal with respect to the “new” labels λ_A, L_A, M_A and are normalized to 1, if one chooses

$$\mathcal{N}_A = \left[\frac{N!(\alpha + \beta + 2N + 1) \Gamma(\alpha + \beta + N + 1)}{\Gamma(\alpha + N + 1) \Gamma(\beta + N + 1)} \right]^{1/2}, \quad (5-7)$$

where, again, $N \equiv N_A$, $\alpha \equiv \alpha_A$ and $\beta \equiv \beta_A$ are given by Eqs. (3-9). By iterating Eqs. (5-1)-(5-4) and (5-6), for $A-1, A-2, \dots, 2$, we obtain

$$\begin{aligned} |\mathbf{x}^{A-1}| &= \rho_A \cos \chi_A, \\ |\mathbf{x}^{A-2}| &= \rho_A \sin \chi_A \cos \chi_{A-1}, \\ |\mathbf{x}^{A-3}| &= \rho_A \sin \chi_A \sin \chi_{A-1} \cos \chi_{A-2}, \end{aligned} \quad (5-8)$$

$$\begin{aligned} |\mathbf{x}^2| &= \rho_A \sin \chi_A \sin \chi_{A-1} \dots \sin \chi_4 \cos \chi_3, \\ |\mathbf{x}^1| &= \rho_A \sin \chi_A \sin \chi_{A-1} \dots \sin \chi_4 \sin \chi_3, \\ d\Omega_A &= \sin^2 \chi_3 \cos^2 \chi_3 d\chi_3 \prod_{i=4}^A \cos^2 \chi_i (\sin^2 \chi_i)^{3i-7} d\chi_i \prod_{j=1}^{A-1} d\Omega(\mathbf{x}^j), \end{aligned}$$

with $0 < \chi_i < \pi/2$, $i = 3, 4, \dots, A$.

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