

ON COLLECTIVE OCTUPOLE DEGREES OF FREEDOM — NEXT PIECES OF THE FORMAL BACKGROUND*

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*Dedicated to Professor Krzysztof Pomorski on the occasion
of the 50th anniversary of his scientific activity*

The concept of an intrinsic system can be extended to the case of collective octupole degrees of freedom by exploiting the symmetry properties with respect to transformations of the octahedral group O_h . Explicit formulas for scalar invariants as polynomials of intrinsic variables are presented. A method of constructing a basis in the space of functions on the octupole intrinsic space is proposed.

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1. Introduction

The role played by collective octupole degrees of freedom still attracts attention of both experimental and theoretical nuclear physicists. First of all, one should mention attempts to find nuclei with a static octupole deformation in actinides region [1], however, as well lighter nuclei ($N = 82$) are an interesting subject of spectroscopic studies [2]. On the theoretical side, a proper description of such phenomena is difficult, mainly due to the necessity of considering both quadrupole and octupole deformations, see *e.g.* recent paper [3].

Here, I present an extension of the results of [4, 5] where we introduced the concept of an intrinsic system for the octupole space based on irreducible representations of the octahedral group O_h .

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The paper is organized as follows. After a brief recollection of basic notions and facts about intrinsic octupole introduced in [4, 5], I discuss rotational invariants built from these variables and show that, quite unexpectedly, the two variants of intrinsic variables are not fully equivalent. I then sketch a method of building basis functions in the intrinsic frame which could in further perspective pave the way to a construction of a basis in the full quadrupole plus octupole space.

2. Intrinsic octupole coordinates

Collective octupole degrees of freedom are described by variables which span the seven-dimensional real irreducible representation of the rotation group $SO(3)$ with the parity operation acting as multiplication by -1 . The best known are seven complex variables α_μ , $\mu = -3, \dots, 3$ with the additional condition $\alpha_{-\mu} = (-1)^\mu \alpha_\mu^*$ ensuring that the considered irreducible representation of $SO(3)$ is of a real type. Another choice, also useful in several applications, is to use seven real variables defined as

$$a_0 = \alpha_0, \quad a_m = \sqrt{2} \operatorname{Re} \alpha_m, \quad b_m = \sqrt{2} \operatorname{Im} \alpha_m, \quad m = 1, 2, 3. \quad (2.1)$$

The concept of an intrinsic (of principal axes) frame of reference appeared to be very fruitful in the case of quadrupole variables, however, extending of this concept to the octupole case is not straightforward. To define an intrinsic system for the octupole space, we exploit properties of octupole variables with respect to the octahedral group $O_h \subset O(3)$, for more details see [4, 5]. This group leaves invariant a set of three intersecting perpendicular lines (without fixed directions and labels) which seems to be a fundamental property of a reference frame. The octupole space can be decomposed as $A_2^- \oplus F_1^- \oplus F_2^-$ of irreducible representations of O_h , with dimensions 1, 3, 3, respectively, see [6]. Coordinates compatible with this decomposition are denoted as $(b, \mathbf{f}, \mathbf{g}) = (b, f_x, f_y, f_z, g_x, g_y, g_z)$, where $b, f_k, g_k, k = x, y, z$ span representations A_2^-, F_1^-, F_2^- , respectively. Explicit expressions for them are given *e.g.* in Appendix B of [5].

In [4, 5], we introduced two variants of the intrinsic system: F_1^- -type and F_2^- -type. In the case of F_1^- variant instead of the LAB system $(b, \mathbf{f}, \mathbf{g})$ variables, one uses $(b', \mathbf{f}', \boldsymbol{\omega})$ variables where $\boldsymbol{\omega}$ are the Euler angles of the rotation such that the result of this rotation has the form of $(b', \mathbf{f}', 0)$. The F_2^- case is defined analogously, with \mathbf{f} and \mathbf{g} interchanged. We presented detailed consequences of this change of variables, in particular we discussed the Hamiltonian and the angular momentum operator expressed through intrinsic variables. It appears, however, a bit surprisingly, that the F_1^- and F_2^- variants are not equivalent, in particular the F_2^- variant does not cover the whole octupole space, as will be shown in Section 3. In the following,

I drop primes and denote intrinsic coordinates as $(b, \mathbf{f}, \boldsymbol{\omega})$. The (b, \mathbf{f}) , $\boldsymbol{\omega}$ will be called the deformation and rotation part, respectively, of octupole variables.

3. Rotational invariants

Of particular importance in the analysis of functions of collective variables are the simplest building blocks of a given multipolarity, in other words, the simplest polynomials (of a given multipolarity) built from the variables. For example, in the quadrupole case, all scalar polynomials can be built from two well-known invariants β^2 , $\beta^3 \cos 3\gamma$. The octupole case is more difficult. Exploiting the connection between invariants of binary forms, see *e.g.* [7] and scalar polynomials of multipole tensors, one finds that in the octupole case there are 4 elementary scalars of the order of 2, 4, 6 and 10, which generate the full ring of polynomial scalars. Moreover, there is also a pseudoscalar polynomial of the order of 15. For details, see [8], where the laboratory frame was discussed. The scalars, denoted here by $\eta_{2,4,6,10}$, can be expressed through couplings of the α variables as follows:

$$\eta_2 = -\sqrt{7} [\alpha\alpha]^0, \quad (3.1)$$

$$\eta_4 = \alpha^{4[2,3,0]}, \quad (3.2)$$

$$\eta_6 = \alpha^{6[2,1,2,3,0]}, \quad (3.3)$$

$$\eta_{10} = \alpha^{10[2,1,2,1,2,1,2,3,0]}, \quad (3.4)$$

where $\alpha^{4[2,3,0]} = [[[\alpha\alpha]^2\alpha]^3\alpha]^0$. The analogous notation is used in (3.3), (3.4). Below, we show explicit formulas for elementary scalars for both F_1^- and F_2^- variants of the intrinsic frame.

F_1^- variant.

$$\eta_2 = b^2 + f_x^2 + f_y^2 + f_z^2 = b^2 + \sigma_2, \quad (3.5)$$

$$\eta_4 = \frac{1}{84\sqrt{5}} \left(16\sigma_4 - 13\sigma_{42} + 80b^2\sigma_2 + 24\sqrt{15}b\sigma_3 \right), \quad (3.6)$$

$$\begin{aligned} \eta_6 = & \frac{\sqrt{3}}{196} \left((11\sigma_2\sigma_{42} - 15\sigma_3^2) - \frac{16}{5}\sigma_2^3 \right) - \frac{1}{7\sqrt{5}}b\sigma_3\sigma_2 \\ & + \frac{1}{196\sqrt{3}}b^2(32\sigma_2^2 - 129\sigma_{42}) + \frac{2\sqrt{5}}{7}b^3\sigma_3 - \frac{20}{147\sqrt{3}}b^4\sigma_2, \end{aligned} \quad (3.7)$$

$$\begin{aligned}
9604 \eta_{10} = & -\frac{400}{9\sqrt{3}} b^8 \sigma_2 + \frac{184\sqrt{5^3}}{3} b^7 \sigma_3 - \frac{5}{\sqrt{3^3}} b^6 (64\sigma_2^2 + 673\sigma_{42}) \\
& + \frac{2092\sqrt{5}}{3} b^5 \sigma_3 \sigma_2 + \frac{1}{\sqrt{3}} b^4 (32\sigma_2^3 - 715\sigma_{42}\sigma_2 - 2289\sigma_3^2) \\
& + \frac{16}{\sqrt{5}} b^3 \sigma_3 (5\sigma_2^2 + 67\sigma_{42}) + \frac{\sqrt{3}}{5} b^2 (192\sigma_2^4 - 439\sigma_{42}\sigma_2^2 - 691\sigma_3^2\sigma_2 - 270\sigma_{82}) \\
& - \frac{3}{\sqrt{5}} b \sigma_3 (84\sigma_2^3 - 259\sigma_{42}\sigma_2 + 255\sigma_3^2) \\
& - \frac{3\sqrt{3}}{100} (576\sigma_2^5 - 2700\sigma_{42}\sigma_2^3 + 2025\sigma_{82}\sigma_2 + 7350\sigma_3^2\sigma_2^2 - 1625\sigma_3^2\sigma_{42}) , \quad (3.8)
\end{aligned}$$

where auxiliary symmetric functions of f_x, f_y, f_z are defined as

$$\sigma_2 = f_x^2 + f_y^2 + f_z^2, \quad \sigma_3 = f_x f_y f_z, \quad (3.9)$$

$$\sigma_4 = f_x^4 + f_y^4 + f_z^4, \quad \sigma_{42} = f_x^2 f_y^2 + f_y^2 f_z^2 + f_x^2 f_z^2, \quad (3.10)$$

$$\sigma_6 = f_x^6 + f_y^6 + f_z^6, \quad \sigma_{82} = f_x^4 f_y^4 + f_y^4 f_z^4 + f_x^4 f_z^4. \quad (3.11)$$

F_2^- variant.

$$\eta_2 = b^2 + g_x^2 + g_y^2 + g_z^2 = b^2 + \tau_2, \quad (3.12)$$

$$\eta_4 = \frac{5\sqrt{5}}{28} \tau_{42}, \quad (3.13)$$

$$\eta_6 = \frac{25\sqrt{3}}{196} \left(3\tau_3^2 - \frac{1}{3} (b^2 + \tau_2) \tau_{42} \right), \quad (3.14)$$

$$\begin{aligned}
9604 \eta_{10} = & -\frac{125}{3^{3/2}} \left[b^6 \tau_{42} + 3b^4 (\tau_2 \tau_{42} - 9\tau_3^2) + 3b^2 (\tau_2^2 \tau_{42} + 2\tau_{42}^2 - 15\tau_3^2 \tau_2) \right. \\
& \left. - 9b \tau_{63} \tau_3 + \left(\tau_2^3 \tau_{42} + \frac{33}{4} \tau_{42}^2 \tau_2 - 9\tau_3^2 \left(4\tau_2^2 - \frac{3}{4} \tau_{42} \right) \right) \right], \quad (3.15)
\end{aligned}$$

where symmetric functions of g_x, g_y, g_z are defined as:

$$\tau_2 = g_x^2 + g_y^2 + g_z^2, \quad \tau_3 = g_x g_y g_z, \quad (3.16)$$

$$\tau_{42} = g_x^2 g_y^2 + g_y^2 g_z^2 + g_x^2 g_z^2, \quad \tau_{63} = (g_z^2 - g_x^2) (g_z^2 - g_y^2) (g_y^2 - g_x^2). \quad (3.17)$$

One should remember that the generators of the ring of invariants (in the polynomial sense) are not uniquely defined. First, they can be multiplied by real numbers. Second, *e.g.* by adding the product $\eta_2 \eta_4$ to η_6 , we obtain again a sixth order scalar (with respect to rotations).

As a simple exercise in the application of invariants, one can check that a point which in the LAB system has coordinates $(b = 0, 0, 0, f_z \neq 0, 0, 0, 0)$ and is trivially described in the F_1^- intrinsic system does not belong to the space of the F_2^- system. The values of invariants do not depend on the choice of the coordinate system and by applying formulas (3.5)–(3.7) and (3.12)–(3.14), we obtain an evident contradiction $\tau_3^2 = -\frac{64}{3375}f_z^6$. Similar considerations show that the set of points of the octupole space which are not covered by the F_2^- is even larger than discussed in this paragraph.

4. Basis in the intrinsic space

In order to apply the presented formalism in the nuclear theory, *e.g.* for study of Hamiltonian and other operators, one requires one more important component, namely an appropriate basis in the Hilbert space of functions defined on the octupole space. Again, the construction of such a basis is more difficult than in the quadrupole case, where several approaches were successfully applied [9]. As can be seen in [8], building eigenfunctions of the harmonic oscillator which have good angular momentum numbers is very difficult even in the laboratory system. Here, I follow the general idea of the method applied in [10] for the quadrupole case which can be summarized as follows. From a properly chosen dense (in the sense of the Hilbert space) set of functions of the intrinsic octupole variables, one constructs a subspace of functions which fulfill two conditions. First (A), they are invariant with respect to the action of the octahedral group. Second (B), they belong to the domain of the Laplace–Beltrami operator which is compatible with the scalar product induced in the intrinsic system by the standard Cartesian scalar product in the laboratory system. From the physical point of view, this operator is (up to a constant factor) the simplest form of the kinetic energy operator in the intrinsic system, see [4, 5]. Then, the standard orthonormalization methods can be applied. At present, the above procedure has been applied only to the F_1^- variant, with results presented briefly below.

In the deformation part of the octupole space, we take all polynomials of the (b, \mathbf{f}) variables times the Gaussian factor $\exp(-(b^2 + \mathbf{f}^2)/2)$. Considering a more general exponent, $-c^2(b^2 + \mathbf{f}^2)/2$ does not present any difficulty.

Condition A. Symmetrization.

It turns out that in the symmetrization stage, it is more convenient to use the spherical coordinates for \mathbf{f} , which are denoted by t, ξ_1, ξ_2 . Then the basic set of functions is organized as follows:

$$b^{n_b} t^{n_t} Y_{lm}(\xi_1, \xi_2) e^{-(b^2 + t^2)/2} \mathcal{D}_{MK}^J(\omega), \quad (4.1)$$

$$N = n_b + n_t, \quad N = 0, 1, 2, \dots, \quad l = n_t, n_t - 2, \dots, 0(1),$$

where \mathcal{D}_{MK}^J are the rotation matrices providing the basis in the $L^2(\text{SO}(3))$ space. One should keep in mind that (lm) indices refer to the group $\text{SO}_A(3)$ generated by operators (4.10) and not the “main” $\text{SO}(3)$ mentioned in Section 2. However, thanks to vector-type properties of the F_1^- IR of the group O_h , the action of this group on the functions $Y_{lm}(\xi_1, \xi_2)$ can be easily determined. Let us add that t and the Gaussian factor are invariant against O_h and b is a pseudoscalar with respect to the O_h action. To obtain O_h -invariant functions from (4.1), we apply the projection operator

$$P_3 P_2 P_1 = (I + R_3 + R_3^2) (I + R_2 + R_2^2 + R_2^3) (I + R_1), \quad (4.2)$$

where $R_k, k = 1, 2, 3$ are well-known generators of O_h , see *e.g.* [11]. If we use $btY\mathcal{D}$ as a shorter notation for (4.1), with the Gaussian factor skipped, we arrive at the formulas

$$P_1 btY\mathcal{D} = bt \left(Y_{lm} \mathcal{D}_{MK}^J + (-1)^{l+J} Y_{l-m} \mathcal{D}_{M-K}^J \right), \quad (4.3)$$

$$P_2 btY\mathcal{D} = [1 + (-1)^{m+K}] \left[1 + (-1)^{n_b + (m+K)/2} \right] btY\mathcal{D}, \quad (4.4)$$

$$P_3 btY\mathcal{D} = bt \sum_{m', K'} \left[\delta_{mm'} \delta_{KK'} + \left(i^{m+K} + (-i)^{m'+K'} \right) \times d_{m'm}^l \left(\frac{\pi}{2} \right) d_{K'K}^J \left(\frac{\pi}{2} \right) \right] Y_{lm'} \mathcal{D}_{MK'}^J, \quad (4.5)$$

where $d_{mn}^l(\theta)$ is the “small” Wigner function. Of course, after the projection, one should choose linearly-independent functions, what is rather easy in the considered case. In particular, one can obtain a simple analytical formula for a number of such functions for given (n_b, n_t, l, J) .

Condition B. Domain of the Laplace–Beltrami operator.

At this stage, we turn back from spherical to Cartesian coordinates for \mathbf{f} . The Laplace–Beltrami operator can be written as (using slightly more compact notation than in [4, 5])

$$\Delta = \frac{1}{d} \frac{\partial}{\partial b} d \frac{\partial}{\partial b} + \sum_{s=x,y,z} \frac{1}{d} \frac{\partial}{\partial f_s} d \frac{\partial}{\partial f_s} + \frac{1}{d} \sum_{k,j=1,2,3} W_k d M_{kj} W_j, \quad (4.6)$$

where

$$d = 8 \left(b^3 - \left(\frac{15}{16} \right) b (f_x^2 + f_y^2 + f_z^2) + 2 \left(\frac{15}{16} \right)^{3/2} f_x f_y f_z \right) \quad (4.7)$$

is the deformation part of the Jacobian of the change of variables (from the laboratory system to the intrinsic system, [5], Eq. (13)) and

$$M = 4 \begin{pmatrix} 16b^2 + 15(f_y^2 + f_z^2) & 15f_x f_y + 8\sqrt{15}b f_z & 8\sqrt{15}b f_y + 15f_x f_z \\ 15f_x f_y + 8\sqrt{15}b f_z & 16b^2 + 15(f_x^2 + f_z^2) & 8\sqrt{15}b f_x + 15f_y f_z \\ 8\sqrt{15}b f_y + 15f_x f_z & 8\sqrt{15}b f_x + 15f_y f_z & 16b^2 + 15(f_x^2 + f_y^2) \end{pmatrix}^{-1}, \quad (4.8)$$

$$W_k = S_k(\boldsymbol{\omega}, \partial_{\boldsymbol{\omega}}) + \Lambda_k(\mathbf{f}, \partial_{\mathbf{f}}), \quad k = 1, 2, 3, \quad (4.9)$$

with

$$\Lambda_1 = 3(f_y \partial_{f_z} - f_z \partial_{f_y})/2, \quad \text{etc.} \quad (4.10)$$

and with S_k being components of the angular momentum multiplied by i (see [5], Eq. (16)).

It can be verified that the functions obtained through symmetrization in the previous stage, denoted as

$$G(b, \mathbf{f}, \boldsymbol{\omega}) e^{-(t^2 + b^2)/2}$$

belong to the domain of Δ provided that

$$d^2 \sum_{\beta=b, \mathbf{f}} \partial_{\beta} (d \partial_{\beta} G) + d \sum_{kj} W_k (d^2 M_{kj} W_j G) - \sum_{kj} (W_k d) d^2 M_{kj} W_j G \quad (4.11)$$

can be expressed as

$$d^3 p(b, \mathbf{f}), \quad (4.12)$$

where p is a polynomial (0 non excluded). This condition is far from trivial, even for low values of N (the order of G in the (b, \mathbf{f}) variables), say $N = 4$, we have to deal with polynomials of the order greater than 10. Hence, to find linear combination of the symmetrized functions that fulfill condition B, I have used the Maxima system for symbolic computations. The developed procedures can be applied for $N \leq 10$, $J \leq 12$ but, at present, the more detailed analysis has been done for N up to 4 and J up to 6.

A few remarks and examples.

1. $J = 0$. For even N , conditions A and B are fulfilled by polynomials $\eta_2^{N/2} = (b^2 + \mathbf{f}^2)^{N/2}$ from which one can easily build Laguerre polynomials $L_{N/2}^{(5/2)}$, which enter the eigenfunctions of the octupole harmonic oscillator with the seniority number $\lambda = 0$, see [8].
2. $N = 4, J = 0$. In this case, we have 5 functions after stage A from which 2 linear combinations fulfilling condition B can be built. One is, as expected, proportional to η_2^2 , while the second one is proportional to η_4 , Eq. (3.6). This is again a nontrivial fact, because this result is obtained in a way that is completely independent from the theory applied in Section 3.

3. The rotation part of the basis functions is conveniently expressed using the semi-Cartesian Wigner functions, see [5], Eq. (8)

$$D_{MK}^{J(+)} = (\mathcal{D}_{MK}^J + (-1)^K \mathcal{D}_{M,-K}^J) / \sqrt{2(1+\delta_{K0})}, \quad K \geq 0, \quad (4.13)$$

$$D_{MK}^{J(-)} = i (\mathcal{D}_{MK}^J - (-1)^K \mathcal{D}_{M,-K}^J) / \sqrt{2}, \quad K > 0. \quad (4.14)$$

For example, in the case of $N = 2, J = 2$, there is only one basis function which can be written as

$$\Psi_{2M}^2 = \sum_{K=0}^2 C_K^{(+)} D_{MK}^{2(+)} + \sum_{K=1}^2 C_K^{(-)} D_{MK}^{2(-)}, \quad (4.15)$$

with

$$C^{(+)} = \left\{ 2f_z^2 - f_y^2 - f_x^2, \left(\sqrt{3}f_x f_z + 4\sqrt{5}b f_y \right) / 2, -\sqrt{3}(f_y - f_x)(f_y + f_x) \right\}, \quad (4.16)$$

$$C^{(-)} = \left\{ \sqrt{3}f_y f_z + 4\sqrt{5}b f_x, -4\sqrt{5}b f_z - \sqrt{3}f_x f_y \right\}. \quad (4.17)$$

5. Concluding remarks

The results presented in this contribution extend our knowledge on the formal properties of the intrinsic system for the octupole tensors. However, there are still problems which remain only partly solved. Let us mention two of them. First, despite some hints, there is no formal proof that the variables chosen according to the F_1^- variant cover the whole octupole space. Second, the integration measure in the deformation part contains the factor $|d| = |8(b^3 - (15/16)b(f_x^2 + f_y^2 + f_z^2) + 2(15/16)^{3/2}f_x f_y f_z)|$ which seems to make it impossible to obtain analytical results for a scalar product of even the simplest basis functions and requires a very careful numerical treatment. On the other hand, limitations on N and J for the basis discussed in Section 4 seem to be not very important for physical applications and, moreover, with some more work, the upper limits can be raised.

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