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ON THE COLLECTIVE OCTUPOLE DEGREES OF FREEDOM*

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The collective octupole degrees of freedom are considered. The spherical components of a real, electric octupole tensor are treated as collective octupole laboratory coordinates. Decomposition of the octupole irreducible representation of orthogonal group O(3) onto three irreducible representations of the cubic $\mathrm{O_h}$ group is presented. Intrinsic cubic coordinates are introduced. The two $\mathrm{O_h}$-symmetric intrinsic coordinate frames are defined. Relations between the laboratory coordinates and the intrinsic cubic ones are discussed in the two cases of intrinsic frame. Operator of the angular momentum and Hamiltonian for the octupole motion are given and expressed in terms of both sets of the intrinsic coordinates. Differences between description of the octupole and the quadrupole degrees of freedom are concluded.

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1. Introduction

Since an early paper by Bohr [1] up to the present time, a definite multipolarity has been attributed to a specific type of nuclear collective excitations. The lowest collective excitations of even–even nuclei have been identified as the quadrupole ones and described successfully until now by the Bohr Hamiltonian [1] generalized over the course of time [2–4]. Nowadays, methods of description of the quadrupole degrees of freedom, and

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structure and parametrization of the quadrupole collective Hamiltonian are known in detail (*cf. e.g.* [5]). Collective excitations of the higher, octupole multipolarity have been also observed for a long time. Recently, thanks to a development of sophisticated experimental techniques, there were several experimental attempts to find nuclei with a static octupole deformation [6, 7]. On the other hand, theoretical treatment of the octupole degrees of freedom is much less developed than that of quadrupole collective variables (see [8] for a review). It seems to be a common opinion that excitations of higher multipolarities, the octupole in particular, can be described in imitation of the quadrupole ones. However, the problem is much more complicated, indeed. One way of the description of the octupole excitations is to attach them to the quadrupole degrees of freedom and enlarge the number of intrinsic variables to $2 + 7 = 9$ [9, 10]. Another method is to describe the quadrupole and the octupole motion separately, and couple them to each other afterwards. Here, we aim at developing methods of description of the octupole mode which turn out to be more complicated than those of the quadrupole case. Definition itself of the so-called intrinsic frame and intrinsic variables is not so obvious [11]. We propose two variants of choice of the intrinsic system based on two different irreducible representations of the group $\mathrm{O_h}$, which exist in the space of octupole variables. We discuss relations between variables in the laboratory and intrinsic frames. Then, we present a construction of operators of the angular momenta and energy (Hamiltonian) in the intrinsic frame.

2. Octupole collective coordinates

2.1. Laboratory and intrinsic coordinates

We assume that the octupole collective coordinates form a real octupole electric (of negative parity) tensor $\boldsymbol{\alpha}_3$. Let the spherical components of tensor $\boldsymbol{\alpha}_3$ in the laboratory frame $\mathrm{U_{lab}}$ (laboratory components) be $\alpha_{3\mu}$ ($\mu = -3, \ldots, 3$). We introduce another frame of reference, $\mathrm{U_{in}}$, called intrinsic frame. We will use the real and imaginary parts, $a_{3\mu}$ and $b_{3\mu}$, respectively, of the intrinsic spherical components as variables instead of the spherical components themselves. Then relation between the laboratory and intrinsic coordinates takes the following form:

$$\alpha_{3\mu} = D^{(+)}_{\mu 0}(\omega) a_{30} + \sum_{k=1,2,3} \left[D^{(+)}_{\mu k}(\omega) a_{3k} + D^{(-)}_{\mu k}(\omega) b_{3k} \right] , \qquad (2.1)$$

where the Euler angles $\omega = (\varphi, \vartheta, \psi)$ define the orientation of the intrinsic frame $\mathrm{U_{in}}$ with respect to the laboratory frame $\mathrm{U_{lab}}$, the semi-Cartesian Wigner functions

$$
\begin{aligned}
D^{(+)}_{\mu k}(\omega) &= \frac{1}{\sqrt{2(1+\delta_{k0})}}\left[\mathcal{D}^3_{\mu k}(\omega)+(-1)^k\mathcal{D}^3_{\mu -k}(\omega)\right], \\
D^{(-)}_{\mu k}(\omega) &= \frac{i}{\sqrt{2}}\left[\mathcal{D}^3_{\mu k}(\omega)-(-1)^k\mathcal{D}^3_{\mu -k}(\omega)\right]
\end{aligned}
\tag{2.2}
$$

form, like the original Wigner functions $\mathcal{D}^3_{\mu k}(\omega)$ [12], still a unitary set.

Intrinsic frame $\mathrm{U_{in}}$ can be defined by three, properly chosen conditions for $a_{3\mu}$ and $b_{3\mu}$, namely

$$
\Lambda_i(a_3(\omega,\alpha_{3\mu}), b_3(\omega,\alpha_{3\mu})) = \Lambda_i(\omega,\alpha_{3\mu}) = 0 \tag{2.3}
$$

for $i = 1, 2, 3$, which determine the Euler angles, $\omega = (\varphi, \vartheta, \psi)$, or, in other words, an orientation of axes of $\mathrm{U_{in}}$ with respect to the axes of $\mathrm{U_{lab}}$. Remaining four independent intrinsic variables are called octupole deformations.

2.2. Cubic intrinsic coordinates

Tensor octupole (3^-) representation of the O(3) orthogonal group can be decomposed onto three irreducible representations of the $\mathrm{O_h}$ cubic holohedral group: one-dimensional denoted as A_2^-, and two three-dimensional, F_1^- and F_2^-, respectively [13]. The sum on the right-hand side of (2.1) can be regrouped according to the $\mathrm{O_h}$ group of transformations of the intrinsic system in the following way:

$$
\alpha_{3\mu} = A_\mu(\omega)b + \sum_{s=x,y,z}\left[F_{\mu s}(\omega)f_s + G_{\mu s}(\omega)g_s\right], \tag{2.4}
$$

where the cubic Wigner functions $A_\mu(\omega)$, $F_{\mu s}(\omega)$, $(s = x, y, z)$ and $G_{\mu s}(\omega)$, $(s = x, y, z)$ are just the $\mathrm{O_h}$ irreps A_2^-, F_1^- and F_2^-, respectively. They are the following combinations of the semi-Cartesian Wigner functions:

$$
\begin{aligned}
A_\mu(\omega) &= D^{(-)}_{\mu 2}(\omega), \\
F_{\mu x}(\omega) &= \sqrt{\tfrac{3}{8}}D^{(+)}_{\mu 1}(\omega) - \sqrt{\tfrac{5}{8}}D^{(+)}_{\mu 3}(\omega), \\
F_{\mu y}(\omega) &= \sqrt{\tfrac{3}{8}}D^{(-)}_{\mu 1}(\omega) + \sqrt{\tfrac{5}{8}}D^{(-)}_{\mu 3}(\omega), \\
F_{\mu z}(\omega) &= D^{(+)}_{\mu 0}(\omega), \\
G_{\mu x}(\omega) &= \sqrt{\tfrac{5}{8}}D^{(+)}_{\mu 1}(\omega) + \sqrt{\tfrac{3}{8}}D^{(+)}_{\mu 3}(\omega), \\
G_{\mu y}(\omega) &= -\sqrt{\tfrac{5}{8}}D^{(-)}_{\mu 1}(\omega) + \sqrt{\tfrac{3}{8}}D^{(-)}_{\mu 3}(\omega), \\
G_{\mu z}(\omega) &= D^{(+)}_{\mu 2}(\omega).
\end{aligned}
\tag{2.5}
$$

The cubic Wigner functions form a unitary set.

The octupole intrinsic cubic coordinates appearing in Eq. (2.4) read:

$$\begin{aligned} b &= b_{32}\,, \\ f_x &= \sqrt{\tfrac{3}{8}}a_{31} - \sqrt{\tfrac{5}{8}}a_{33}\,, \qquad f_y = \sqrt{\tfrac{3}{8}}b_{31} + \sqrt{\tfrac{5}{8}}b_{33}\,, \qquad f_z = a_{30}\,, \\ g_x &= \sqrt{\tfrac{5}{8}}a_{31} + \sqrt{\tfrac{3}{8}}a_{33}\,, \qquad g_y = -\sqrt{\tfrac{5}{8}}b_{31} + \sqrt{\tfrac{3}{8}}b_{33}\,, \qquad g_z = a_{32}\,. \end{aligned} \tag{2.6}$$

3. Octupole deformations

Point group $\mathrm{O_h}$ is a natural symmetry group of the three-dimensional coordinate system because the forty eight group elements are: the eight reverses of the axis arrows for each out of six permutations of axes. Three Bohr's rotations, R_1, R_2, R_3, and inversion P can serve as generators of this group (see [5]). A natural way to define the intrinsic frame, which conserve the $\mathrm{O_h}$-symmetry, is to take the three functions, Λ_i of Eq. (2.3), equal to three cubic coordinates (2.6), which belong to one three-dimensional representation of $\mathrm{O_h}$. There are two such possibilities in our case. We shall investigate both of them.

3.1. F_1^--covariant deformations

One of the two possible $\mathrm{O_h}$ covariant definitions of the intrinsic frame is to take Eq. (2.3) in the following form:

$$\Lambda_s(b,f,g) = g_s = 0 \quad \text{for} \quad s = x,y,z\,. \tag{3.1}$$

Then, instead of using the seven laboratory collective coordinates, $\alpha_{3\mu}$, we use the three Euler angles φ, ϑ, ψ, which define orientation of the body with respect to the laboratory frame, and the four octupole deformations b, $f = (f_x, f_y, f_z)$. The transformation from the intrinsic to the laboratory coordinates looks as follows:

$$\alpha_{3\mu}(\omega,b,f) = A_\mu(\omega)b + \sum_{s=x,y,z} F_{\mu s}(\omega) f_s\,. \tag{3.2}$$

Jacobian of the transformation is equal to

$$\begin{aligned} D_f(\vartheta,b,f_x,f_y,f_z) &= 8\sin\vartheta \left[b\left(b^2 - \tfrac{15}{16}\left(f_x^2+f_y^2+f_z^2\right)\right) + \tfrac{15}{8}\sqrt{\tfrac{15}{16}} f_x f_y f_z \right] \\ &= 8\sin\vartheta W_f(b,f)\,. \end{aligned} \tag{3.3}$$

Transformation (3.2) is reversible for the deformations contained inside hyper-surface $D_f(\vartheta,b,f_x,f_y,f_z) = 0$. Since the F_1^--covariant (vector) deformations (f_x, f_y, f_z) are transformed under the $\mathrm{O_h}$ transformations of the intrinsic frame-like coordinates x, y, z, it follows directly from the O_h symmetry that it is sufficient to consider only non-negative values of them, that is $f_x, f_y, f_z \geq 0$. Deformation b is invariant under rotations R_1 and R_3, and changes the sign under R_2 and inversion P. However, it is not so simple to determine the range of b because it depends on values of f.

3.2. F_2^--covariant deformations

Another possible O_h covariant definition of the intrinsic frame is the following:

$$f_s = 0 \quad \text{for} \quad s = x, y, z \,. \tag{3.4}$$

Then, the intrinsic coordinates are: the three Euler angles φ, ϑ, ψ, which define orientation of the new intrinsic with respect to the laboratory frame, and the four octupole deformations b and $g = (g_x, g_y, g_z)$ and the transformation from the intrinsic to the laboratory coordinates looks as follows:

$$\alpha_{3\mu}(\omega, b, g) = A_\mu(\omega) b + \sum_{s=x,y,z} G_{\mu s}(\omega) g_s \,. \tag{3.5}$$

Jacobian of the transformation is, up to the sign, equal to

$$D_g(\vartheta, b, g) = 15\frac{\sqrt{15}}{4} \sin\vartheta g_x g_y g_z = 15\frac{\sqrt{15}}{4} \sin\vartheta W_g(b, g) \tag{3.6}$$

and does not depend on b. Obviously, transformation (3.5) is reversible in full quadrant $g_x > 0,\ g_y > 0,\ g_z > 0$. Transformation rules of deformations g under O_h are a bit different from those for f: $g_x,\ g_y,\ g_z$ are transformed under R_1-, R_3- and P-like coordinates $x,\ y,\ z$, while they change additionally the sign under R_2. It follows from the symmetry conditions that it is sufficient to take non-negative values of b only.

4. Octupole collective Hamiltonian

4.1. General structure

The collective octupole Hamiltonian, which is a second-order differential operator in coordinates $\alpha_{3\mu}$, invariant under rotations and reflection in the physical space, real and Hermitian with weight $W(\boldsymbol{\alpha}_3)$, takes the following general form (*cf.* [5]):

$$H(\boldsymbol{\alpha}_3, \boldsymbol{\partial\alpha}_3) = -\frac{1}{2W(\boldsymbol{\alpha}_3)} \sum_{\mu,\nu} \frac{\partial}{\partial\alpha_{3\mu}} W(\boldsymbol{\alpha}_3) B^{-1}_{3\mu 3\nu}(\boldsymbol{\alpha}_3) \frac{\partial}{\partial\alpha_{3\nu}} + V(\boldsymbol{\alpha}_3)\,, \tag{4.1}$$

where $B_{3\mu 3\nu}(\boldsymbol{\alpha}_3)$ is an octupole inertial bitensor fulfilling the following relation:

$$\sum_{\nu} B^{*}_{3\mu 3\nu}(\boldsymbol{\alpha}_3) B^{-1}_{3\nu 3\mu'}(\boldsymbol{\alpha}_3) = \delta_{\mu\mu'} \tag{4.2}$$

and $V(\boldsymbol{\alpha}_3)$ is a potential. When Hamiltonian (4.1) comes from a classical one by quantization, the weight is $W(\boldsymbol{\alpha}_3) = \sqrt{\det\left(B_{3\mu 3\nu}(\boldsymbol{\alpha}_3)\right)}$.

For the Hamiltonian to be Hermitian and even, the octupole bitensor, $B_{3\mu 3\nu}(\boldsymbol{\alpha}_3)$ should be symmetric in μ and ν and should have positive parity. Thus, it can be presented in the following form:

$$B_{3\mu 3\nu}(\boldsymbol{\alpha}_3) = \sum_{\lambda=0,2,4,6} (3\mu 3\nu|\lambda\kappa)\tau_{\lambda\kappa}(\boldsymbol{\alpha}_3)\,, \tag{4.3}$$

where all the four tensors $\boldsymbol{\tau}_\lambda$ are even and isotropic functions of $\boldsymbol{\alpha}_3$. Since tensor $\boldsymbol{\tau}_\lambda$ possesses $2\lambda+1$ components, bitensor $B_{3\mu 3\nu}$ has 28 components. The question is whether these components are all independent. To answer the question, one should construct and parametrize tensors $\boldsymbol{\tau}_\lambda$ [14]. All these tensors can be presented in the form of a linear combination of a number of fundamental tensors of a given rank λ with arbitrary scalar coefficients. There are four elementary scalars of the order of two, four, six and ten in $\alpha_{3\mu}$, respectively. We have five even fundamental tensors of rank $\lambda = 2$, nine for $\lambda = 4$ and fourteen for $\lambda = 6$. These latter are connected with each other through a sixteenth-order syzygy. Hence, the inertial bitensor is parametrized by 28 scalar functions at least and its components can all be independent.

As a scalar, Hamiltonian (4.1) commutes with the angular momentum of the octupole motion [9] which is equal to

$$L^{(3)}_{1\kappa}(\boldsymbol{\alpha}_3, \boldsymbol{\partial\alpha}_3) = -2\sqrt{7}\sum_{\mu\nu}(3\mu 3\nu|1\kappa)\alpha_{3\mu}\frac{\partial}{\partial\alpha^{*}_{3\nu}}\,. \tag{4.4}$$

4.2. Hamiltonian in the intrinsic coordinates

A bit tedious calculation, which are not to be presented here, allows us to express derivatives with respect to the laboratory coordinates by those with respect to the Euler angles and deformations in a given intrinsic system. As can be expected, independently of a choice of the intrinsic system, the components of angular momentum of Eq. (4.4) can be expressed as

$$\begin{aligned} L^{(3)}_{1\kappa} \;=\; & \mathcal{D}^{1}_{\kappa 0}(\omega) L_z(\omega, \partial/\partial\omega) \\ & -\frac{1}{\sqrt{2}}\left[\left(\mathcal{D}^{1}_{\kappa 1}(\omega) - \mathcal{D}^{1}_{\kappa -1}(\omega)\right) L_x(\omega, \partial/\partial\omega)\right. \\ & \left. +i\left(\mathcal{D}^{1}_{\kappa 1}(\omega) + \mathcal{D}^{1}_{\kappa -1}(\omega)\right) L_y(\omega, \partial/\partial\omega)\right]\,, \end{aligned} \tag{4.5}$$

where the Cartesian components L_x, L_y, L_z depend on the Euler angles and their derivatives only and are given by standard formulae [15].

It is convenient to transform the octupole Hamiltonian to the intrinsic frame to have insight into types of the octupole excitations. To this end, let us take the simplest octupole Hamiltonian to observe inherent characteristics of the octupole motion. The kinetic energy has the simplest form when we take only the first term in sum of equation (4.3) and put scalar τ_0 equal to a constant, namely

$$B_{3\mu 3\nu}(\boldsymbol{\alpha}_3) = -\sqrt{7}(3\mu 3\nu|00)B = (-1)^{\mu}\delta_{\mu-\nu}B \tag{4.6}$$

which is the Bohr original inertial bitensor with mass parameter B. Then the Hamiltonian takes the following form:

$$H(\boldsymbol{\alpha}_3, \boldsymbol{\partial\alpha}_3) = -\frac{1}{2B}\sum_{\mu}\frac{\partial}{\partial\alpha_{3\mu}}\frac{\partial}{\partial\alpha^*_{3\mu}} + V(\boldsymbol{\alpha}_3)\,. \tag{4.7}$$

For both intrinsic frames defined by (3.1) and (3.4), respectively, Hamiltonian (4.7) is presented in the following form:

$$\begin{aligned} H(b,d,\omega) \;=\; & -\frac{1}{2BW_d(b,d)}\left\{\frac{\partial}{\partial b}W_d(b,d)\frac{\partial}{\partial b} + \sum_s \frac{\partial}{\partial d_s}W_d(b,d)\frac{\partial}{\partial d_s}\right.\\ & -\sum_{s,t}\Big(L_s(\omega,\partial/\partial\omega) - J_s^{(d)}(d,b,\partial d,\partial b)\Big)\,W_d(b,d)\left(\hat{I}^{(d)}(b,d)\right)^{-1}_{st}\\ & \left.\times\Big(L_t(\omega,\partial/\partial\omega) - J_t^{(d)}(d,b,\partial d,\partial b)\Big)\right\} + V(b,d)\,, \end{aligned} \tag{4.8}$$

where $J_s^{(d)}(d,b,\partial d,\partial b)$ are components of an intrinsic angular momentum and $\hat{I}^{(d)}(b,d)$ is a matrix (Cartesian tensor) of moments of inertia. Symbol d stands for f or g in the case of the intrinsic frame (3.1) or (3.4), respectively. The potential, being a function of the four elementary scalars, is a function of four octupole deformations $b,\ d$ in the given intrinsic frame.

In the case of the intrinsic frame (3.1), the intrinsic angular momentum and the matrix of moments of inertia read:

$$J_s^{(f)}(f,\partial f) = \frac{3}{2}i\left(f_t\frac{\partial}{\partial f_u} - f_u\frac{\partial}{\partial f_t}\right) \tag{4.9}$$

and

$$\hat{I}^{(f)}(b,f) = \begin{pmatrix} 4b^2 + \frac{15}{4}\left(f_y^2 + f_z^2\right) & \frac{15}{4}f_xf_y + 2\sqrt{15}bf_z & \frac{15}{4}f_xf_z + 2\sqrt{15}bf_y \\ \frac{15}{4}f_xf_y + 2\sqrt{15}bf_z & 4b^2 + \frac{15}{4}\left(f_x^2 + f_z^2\right) & \frac{15}{4}f_yf_z + 2\sqrt{15}bf_x \\ \frac{15}{4}f_xf_z + 2\sqrt{15}bf_y & \frac{15}{4}f_yf_z + 2\sqrt{15}bf_x & 4b^2 + \frac{15}{4}\left(f_x^2 + f_y^2\right) \end{pmatrix}, \tag{4.10}$$

respectively, and in the case of (3.4), we have

$$J_s^{(g)}(g,b,\partial g,\partial b) = -i\left[\tfrac{1}{2}\left(g_t\frac{\partial}{\partial g_u} - g_u\frac{\partial}{\partial g_t}\right) + 2\left(g_s\frac{\partial}{\partial b} - b\frac{\partial}{\partial g_s}\right)\right], \quad (4.11)$$

and

$$\hat{I}^{(f)}(b,g) = \begin{pmatrix} \frac{15}{4}\left(g_y^2+g_z^2\right) & \frac{15}{4}g_xg_y & \frac{15}{4}g_xg_z \\ \frac{15}{4}g_xg_y & \frac{15}{4}\left(g_x^2+g_z^2\right) & \frac{15}{4}g_yg_z \\ \frac{15}{4}g_xg_z & \frac{15}{4}g_yg_z & \frac{15}{4}\left(g_x^2+g_y^2\right) \end{pmatrix}. \quad (4.12)$$

We see that none of intrinsic frames is the system of principal axes of the moment of inertia. The intrinsic octupole motion has its own intrinsic angular momentum, which interacts by the Coriolis and centrifugal forces with the total angular momentum.

In the cases of Hamiltonians with more involved inertial bitensors, the vibration–rotation terms of type

$$i\left(\frac{\partial}{\partial d_s}W_d(b,d)B_{st}^{-1}\left(L_t - J_t^{(d)}\right) - \left(L_t - J_t^{(d)}\right)W_d(b,d)B_{st}^{-1}\frac{\partial}{\partial d_s}\right), \quad (4.13)$$

where B_{st}^{-1} are some inertial functions, can appear.

5. Conclusions

The well-known quadrupole collective motion turns out to be very special and, in spite of common opinions, can hardly serve as a standard for collective motions of higher multipolarities. Differences are essential. The octupole collective motion is much more complicated not only because it has two degrees of freedom more, but because theory of octupole spherical tensors is much more complex.

Principal axes can be defined for a quadrupole tensor. So, the system of principal axes is a natural intrinsic frame for the quadrupole degrees of freedom. Hardly anyone links this definition with the decomposition of the quadrupole tensor components into combinations of cubic symmetry, but in fact, it means vanishing of the only one such three-dimensional combination. There are no principal axes for octupole tensors. Therefore, it remains to define an intrinsic frame for the octupole degrees of freedom according to decomposition onto representations of the cubic holohedral group. There are then two possibilities for the intrinsic frame. No wonder that the moment of inertia is not diagonal in frames defined in such a way. The quadrupole vibrations do not carry any angular momentum. On the other hand, the octupole vibrations produce an intrinsic angular momentum which is coupled to the total angular momentum through the Coriolis and centrifugal forces. Finally, a quadrupole symmetric bitensor have fifteen components but at most six of them can be independent. A consequence of this is that the kinetic energy of the quadrupole motion is always decomposed into three vibrational and three rotational energy terms. However, octupole symmetric tensors have twenty eight components each and all of them can be independent. It means that ten vibrational, six rotational and twelve vibration–rotation terms are all possible in the kinetic energy of octupole motion. In conclusion, we want to stress that describing the octupole excitations, one should be careful with analogies to the quadrupole ones. We should look at the octupole degrees of freedom from a bit different point of view and should learn how to treat them.

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