Parametrization of the octupole degrees of freedom

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A simple parametrization for the octupole collective variables is proposed and the symmetries of the wave functions are discussed in terms of the solutions corresponding to the vibrational limit.
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I. INTRODUCTION

The collective description of the octupole degrees of freedom has been a long standing problem in nuclear physics [1]. The phenomenological description of low-energy vibrational states [2,3] discussed them in terms of simple ''surface modes'' thus allowing for the description of the octupole degrees of freedom in terms of seven collective variables $\alpha_{3\mu}$ [2,4]. In the 1980s, theoretical calculations [5] predicted the existence of octupole stable deformations and this problem aroused considerable interest, especially in the Ce-Ba and the Rn-Th regions. The level scheme of a few moderately or weakly deformed nuclei, such as ^{64}Ge [6], ^{148}Sm [7], ^{218}Ra [8], or ^{233,225}Ra [9] presents features that may be related to octupole instabilities and softness of the nucleus with respect to possible exotic octupole deformations. Lately [10] there has been evidence for the existence of stable octupole deformations in the Rn-Th region making the problem of the collective description of this degree of freedom more actual. It has been shown that this type of collective excitations can significantly change the fusion cross section for heavy ions [11]. Initially, only octupole deformations of the Y_{30} type were considered, but the possibility of other type of deformations (such as Y_{32} [12] or Y_{31} [13]) has also been discussed. The study of more general structures was intended without much success [14]. There were also several proposals related to the appropriate parametrization of the collective variables. Rohozinski [15] proposed a parametrization based on the symmetries coming from the O_h group of transformations of the frame of reference. Hamamoto [16] wrote octupole shapes in terms of the irreducible representations of the octahedron group $A_1, F_1(k)$ and $F_2(k)$ and suggested that a parametrization that covers all possible octupole deformed shapes (without double counting the same shape) is provided by removing $F_2(k)$ (eliminating in this way three parameters).

In the present paper we return to the idea used for the definition of the intrinsic system in Bohr's paper [2] (also used by other authors for the collective description of the pairing degrees of freedom): in the intrinsic system the inertia tensor (related to the rotational part of the kinetic energy) must be diagonal.

In Sec. II we review some features of the collective excitations, the Hamiltonian, we discuss how to separate the rotational and intrinsic degrees of freedom and we propose a simple parametrization. We use the Pauli prescription to quantize the quadratic Hamiltonian. In Sec. III we discuss the structure of the wave functions and of the elementary scalars or invariants (as defined in Ref. [17]), as well as the symmetries of the wave function. In Sec. IV we discuss the rigid rotor that illustrates the differences between the rotational bands related with octupole deformations as compared with the quadrupole ones [18]. Section V summarizes the results obtained in the present paper.

II. FORMULATION OF THE PROBLEM

A. The collective variables

The theory of collective oscillations has been developed a long time ago by several authors [2,3,19]. The classical case corresponds to quadrupole oscillations that were described in detail by Bohr in 1952. A very clear and pedagogical discussion concerning the symmetries and wave functions for this problem can be found in a paper [17] by Kumar and Baranger, where a numerical solution for this problem was first proposed. A collective treatment was also performed for the pairing degrees of freedom: the pairing acting only on one type of particles yields a two dimensional collective description [20], while the corresponding to the $T=1$ case yields a six-dimensional one [21]. In the three cases described, the recipe used to found the collective description has the same basic ingredients.

(a) The kinetic energy was written explicitly in terms of the time derivatives of the collective variables.

(b) The collective variables (of dimension five, two or six, depending on the case) were written in the intrinsic system, isolating the intrinsic variables from those that describe the

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motion of the intrinsic system (the three Euler angles in the five- and six-dimensional cases, one angle in the two dimensional one). In all cases the intrinsic system was defined as the system where the inertia tensor (the part related with collective rotations) were diagonal.

(c) The kinetic energy was written in terms of the Euler angles and the intrinsic variables, and the coupling between both types of degrees of freedom was studied. Regarding the potential energy it has parts that depend only on the collective variables (and not on their time derivatives). This part can be written in terms of elementary scalars [17] that are constructed using the collective variables. For example, in the quadrupole case there are only two of such scalars [β^2 and $\beta^3 \cos(3\gamma)$, using Ref. [2] notation], in the pairing case (between particles of one type) there is only one of such scalars (Δ^2 using Ref. [20] notation) and in the $T=1$ pairing case there are three of such scalars [Δ^2, $\Delta^2 e^{\pm 4i\phi} \cos(2\Gamma)$, using Ref. [21] notation].

(d) The general symmetry properties of the wave functions that are related to different choices of collective (Euler) angles and intrinsic variables corresponding to the same collective variables in the lab system are used to define the range of the different intrinsic variables. In some simple cases it was also possible to write down explicitly some elementary tensors [17,22,23] in terms of the collective variables.

In the present paper we will follow this program for the octupole surface oscillations, relating them to the shape of the nucleus. Many times the surface of the nucleus, in polar coordinates, has been expressed in terms of the nuclear radius as

$$R(\theta,\phi)=R_0\left(1+\sum_{\lambda\mu} \alpha_{\lambda,\mu} Y_{\lambda,\mu}(\theta,\phi)\right), \qquad (2.1)$$

where R_0 is the radius of the nucleus in its spherical equilibrium shape and $\alpha_{\lambda,\mu}$ are the collective coordinates that describe the deformation of the nuclear surface. We use for the $Y_{\lambda,\mu}$ the spherical harmonics satisfying the Condon and Shortley convention, i.e., $Y_{\lambda,-\mu}=(-1)^\mu(Y_{\lambda,\mu})^*$. As the radius has to be real, it follows that $\alpha_{\lambda,-\mu}=(-1)^\mu(\alpha_{\lambda,\mu})^*$.

It is assumed that these variables change slowly with time, and therefore it is usual to express their kinetic energy as a quadratic function of the velocities as

$$\mathcal{T}=\frac{1}{2}\sum_{\lambda\mu} B_\lambda|\dot{\alpha}_{\lambda,\mu}|^2, \qquad (2.2)$$

where $\dot{\alpha}_\mu$ is the time derivative of α_μ. It is well known that the coefficients $\alpha_{\lambda,\mu}$ written in lab system and the $\alpha_{\lambda,\mu}$ written in the intrinsic system (that we will denote by $a_{\lambda,\mu}$ to avoid confusions) are related by (in what follows we use the notation of Ref. [19])

$$a_{\lambda,\mu}=\sum_\nu \mathcal{D}^\lambda_{\mu,\nu}(\omega_i)\alpha_{\lambda,\mu}, \qquad (2.3)$$

where ω_i are the three Euler angles. As usual the $\mathcal{D}^\lambda_{\mu,\nu}(\omega_i)$ functions, which are related to the matrix element of the rotation operation, are defined by

$$\mathcal{D}^\lambda_{\mu,\nu}(\omega_i)=\langle\lambda,\mu|\exp(i\psi I_z)\exp(i\theta I_y)\exp(i\phi I_z)|\lambda,\nu\rangle, \qquad (2.4)$$

where $\omega_i\equiv(\psi,\theta,\phi)$ are the Euler angles.

From Eq. (2.3) it follows that

$$\alpha_{\lambda,\mu}=\sum_\nu [\mathcal{D}^\lambda_{\mu,\nu}(\omega_i)]^* a_{\lambda,\nu}, \qquad (2.5)$$

with $[\mathcal{D}^\lambda_{\mu,\nu}(\omega_i)]^*=(-1)^{\nu-\mu}\mathcal{D}^\lambda_{-\mu,-\nu}(\omega_i)$.

In order to evaluate the kinetic energy we must write down explicitly the time derivative of $\alpha_{\lambda,\mu}$:

$$\dot{\alpha}_{\lambda,\mu}=\sum_\nu [\mathcal{D}^\lambda_{\mu,\nu}(\omega_i)]^*\dot{a}_{\lambda,\nu}+\sum_\nu [\dot{\mathcal{D}}^\lambda_{\mu,\nu}(\omega_i)]^* a_{\lambda,\nu}. \qquad (2.6)$$

The time derivative of the $\mathcal{D}^\lambda_{\mu,\nu}(\omega_i)$ functions can be expressed as

$$\dot{\mathcal{D}}^\lambda_{\mu,\nu}(\omega_i)=i\sum_{m,\kappa} q_\kappa \mathcal{D}^\lambda_{\mu,m}(\omega_i)(M_\kappa)_{\nu,m}, \qquad (2.7)$$

where M_κ are the $(2\lambda+1)$ dimensional representation of the angular momentum operator and satisfy the commutation relations

$$[M_1,M_2]=-iM_3, \qquad (2.8)$$

and cyclic permutations (note the signs). It is customary to use a representation where $(M_3)_{m,n}=m\delta_{m,n}$. The magnitudes q_κ are the angular velocity components in the κ direction. We can then express the kinetic energy as

$$\mathcal{T}=\frac{B}{2}\sum_\mu (\dot{\alpha}_{\lambda,\mu})^*\dot{\alpha}_{\lambda,\mu}=\mathcal{T}_{\text{vibration}}+\mathcal{T}_{\text{rotation}}+\mathcal{T}_{\text{coupling}}, \qquad (2.9)$$

where for simplicity a single λ is considered, and

$$\mathcal{T}_{\text{vibration}}=\frac{B}{2}\sum_{\mu,\nu,\nu'} \mathcal{D}^{\lambda*}_{\mu,\nu}\mathcal{D}^\lambda_{\mu,\nu'}\dot{a}^*_{\lambda,\nu'}\dot{a}_{\lambda,\nu},$$

$$\mathcal{T}_{\text{rotation}}=\frac{B}{2}\sum_{\mu,\nu,\nu',m,m',\kappa,\kappa'} \mathcal{D}^{\lambda*}_{\mu,m}$$
$$\times *\mathcal{D}^\lambda_{\mu,m'}a_{\lambda,\nu}a^*_{\lambda,\nu'}q_\kappa q_{\kappa'}(M_\kappa)_{\nu,m}(M_{\kappa'})_{m',\nu'}, \qquad (2.10)$$

$$\mathcal{T}_{\text{coupling}}=i\frac{B}{2}\sum_{\mu,\nu,\nu',m,\kappa} [-\dot{a}^*_{\lambda,\nu'}a_{\lambda,\nu}\mathcal{D}^{\lambda*}_{\mu,m}\mathcal{D}^\lambda_{\mu,\nu'}q_\kappa(M_\kappa)_{\nu,m}$$
$$+\dot{a}_{\lambda,\nu}a^*_{\lambda,\nu'}\mathcal{D}^{\lambda*}_{\mu,\nu'}\mathcal{D}^\lambda_{\mu,m}q_\kappa(M_\kappa)_{m,\nu}].$$

Using the unitarity condition for the $\mathcal{D}^\lambda_{\mu,\nu}(\omega_i)$ functions $[\Sigma_\mu \mathcal{D}^{\lambda*}_{\mu,\nu}(\omega_i)\mathcal{D}^\lambda_{\mu,\nu'}(\omega_i)=\delta_{\nu,\nu'}]$, the vibrational part of the kinetic energy simplifies to

$$\mathcal{T}_{\text{vibration}}=\frac{B}{2}\sum_\nu \dot{a}^*_{\lambda,\nu}\dot{a}_{\lambda,\nu}, \qquad (2.11)$$

while the rotational part is

$$\mathcal{T}_{\text{rotation}}=\frac{B}{2}\sum_{\kappa,\kappa'} q_\kappa q_{\kappa'}\sum_{\nu,\nu'} a_{\lambda,\nu}a^*_{\lambda,\nu'}(M_\kappa M_{\kappa'})_{\nu,\nu'}$$
$$=\frac{1}{2}\sum_{\kappa,\kappa'} q_\kappa q_{\kappa'}\mathcal{J}_{\kappa\kappa'}, \qquad (2.12)$$

where the inertia tensor is defined as

$$\mathcal{J}_{\kappa\kappa'}=B\sum_{\nu,\nu'} a_{\lambda,\nu}a^*_{\lambda,\nu'}(M_\kappa M_{\kappa'})_{\nu,\nu'}. \qquad (2.13)$$

The coupling between the internal and rotational degrees of freedom maintains a complicated structure, i.e.,

$$\mathcal{T}_{\text{coupling}}=i\frac{B}{2}\sum_{\nu,\nu',\kappa} q_\kappa[\dot{a}_{\lambda,\nu}a^*_{\lambda,\nu'}-\dot{a}^*_{\lambda,\nu'}a_{\lambda,\nu}](M_\kappa)_{\nu,\nu'}$$
$$=i\sqrt{21}B\{\vec{q}\{a_3\dot{a}_3\}^1\}^0_0, \qquad (2.14)$$

where $\{\ \}^J_M$ means the angular momentum coupling to J,M, and the last line corresponds to the $\lambda=3$ case.

B. Definition of the intrinsic system

We now proceed to the definition of the intrinsic system. We have isolated three rotational variables (the Euler angles), but we also have $(2\lambda+1)$ coordinates $a_{\lambda,\nu}$. It is necessary to reduce their number to $(2\lambda-2)$. This is customary achieved by imposing the condition

$$\mathcal{J}_{\kappa\kappa'}=\mathcal{J}_\kappa\delta_{\kappa\kappa'}. \qquad (2.15)$$

In fact, the requirement is that the off-diagonal elements of $\mathcal{J}_{\kappa\kappa'}$ vanish. These three conditions, which usually are non-linear, in principle reduce by three the number of parameters. The inertia tensor $\mathcal{J}_{\kappa\kappa'}$ can be expressed in terms of the coupling to angular momentum two and zero of the collective variables, using the fact that

$$(M_\mu M_{\mu'})_{\nu,\nu'}=\sum_J \langle 1\mu 1\mu'|JM\rangle\{MM\}^J_M. \qquad (2.16)$$

Due to symmetry reasons, the only values of J that survive in the summation related with the inertia tensor are two or zero. For $\lambda=3$ the explicit expressions for the diagonal components of the inertia tensor are the following:

$$\mathcal{J}_1=B[4\sqrt{7}\{aa\}^0_0+\sqrt{21}\{aa\}^2_0-3\sqrt{14}\,\text{Re}\{aa\}^2_2],$$

$$\mathcal{J}_2=B[4\sqrt{7}\{aa\}^0_0+\sqrt{21}\{aa\}^2_0+3\sqrt{14}\,\text{Re}\{aa\}^2_2],$$

$$\mathcal{J}_3=B[4\sqrt{7}\{aa\}^0_0-2\sqrt{21}\{aa\}^2_0], \qquad (2.17)$$

while the vanishing of the off-diagonal components yields[1]

$$\mathcal{J}_{12}=3B\sqrt{14}\,\text{Im}\{aa\}^2_2=0,$$

$$\mathcal{J}_{13}=3B\sqrt{14}\,\text{Re}\{aa\}^2_1=0,$$

$$\mathcal{J}_{23}=3B\sqrt{14}\,\text{Im}\{aa\}^2_1=0. \qquad (2.18)$$

It is convenient to define the auxiliary variables $u_m=\{aa\}^2_m$. The definition of the intrinsic system through the cancellation of the off-diagonal components of the inertia tensor is therefore equivalent to the conditions $u_1=0$, u_2 and u_{-2} real. It must be noted that similar conditions are held in the quadrupole case. In this case those conditions are satisfied if $a_{2,1}=a_{2,-1}=0$ and $a_{2,2}=a_{2,-2}$ and real. In the octupole case, one must satisfy three nonlinear equations, whose solutions are more complicated.

The $a_{3\nu}$ (in what follows we will concentrate on the $\lambda=3$ case, and therefore use a_ν) must be expressed in terms of four independent variables. Calling them X, Y, Z, and γ it is possible to use as a parametrization

$$a_3=\left[\cos\gamma-\frac{\sqrt{3}}{2}\sin\gamma\right]X+i\left[\cos\gamma+\frac{\sqrt{3}}{2}\sin\gamma\right]Y,$$

$$a_2=\frac{1}{\sqrt{2}}\sin\gamma Z,$$

$$a_1=\frac{\sqrt{5}}{2}\sin\gamma[X+iY],$$

$$a_0=\sqrt{5}\cos\gamma Z, \qquad (2.19)$$

that automatically makes the off-diagonal components of the inertia tensor equal to zero.

To simplify the notation we define $x_\kappa=X,Y,Z$ and $\gamma_\kappa=\gamma-\pi/3\kappa$ for $\kappa=1,2,3$. In terms of these variables, the u_m different from zero can be written as

$$u_0=\eta\cos\gamma,$$

$$u_2=\frac{\eta}{\sqrt{2}}\sin\gamma, \qquad (2.20)$$

where $\eta=5\sqrt{2/21}\Sigma_\kappa x^2_\kappa\cos\gamma_\kappa$.

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[1]In the quadrupole case $\mathcal{J}_{12}$ is related to $\text{Im}\{aa\}^2_2$ while $\mathcal{J}_{13}$ and $\mathcal{J}_{23}$ are related to $\{aa\}^2_1$. The diagonal components of the inertia tensor are related to $\{aa\}^0_0$, $\{aa\}^2_0$, and $\text{Re}\{aa\}^2_2$. In a similar way in the $T=1$ pairing collective description the off diagonal components of the inertia tensor can be written as $\mathcal{J}_{12}=-B\text{Im}\{\Delta\Delta^*\}^2_2$, $\mathcal{J}_{13}=-B\text{Re}\{\Delta\Delta^*\}^2_1$, $\mathcal{J}_{23}=-B\text{Im}\{\Delta\Delta^*\}^2_1$. The diagonal components are related to $\{\Delta\Delta^*\}^0_0$, $\text{Re}\{\Delta\Delta^*\}^2_2$, and $\{\Delta\Delta^*\}^0_0$.

TABLE I. The inertia matrix $G_{m,n}$.

	$\dot{X}$	$\dot{Y}$	$\dot{Z}$	$\dot{\gamma}$	q_3	q_2	q_1
$\dot{X}$	$1+4\cos^2\gamma_1$	0	0	$-2X\sin(2\gamma_1)$	$4Y(1+2\cos\gamma_1\cos\gamma_2)$	$-4Z(1+2\cos\gamma_1\cos\gamma_3)$	0
$\dot{Y}$	0	$1+4\cos^2\gamma_2$	0	$-2Y\sin(2\gamma_2)$	$-4Z(1+2\cos\gamma_1\cos\gamma_2)$	0	$4Z(1+2\cos\gamma_2\cos\gamma_3)$
$\dot{Z}$	0	0	$1+4\cos^2\gamma_3$	$-2Z\sin(2\gamma_3)$	0	$4X(1+2\cos\gamma_1\cos\gamma_3)$	$-4Y(1+2\cos\gamma_1\cos\gamma_3)$
$\dot{\gamma}$	$-2X\sin(2\gamma_1)$	$-2Y\sin(2\gamma_2)$	$-2Z\sin(2\gamma_3)$	$\sum_\kappa x_\kappa^2(1+4\sin^2\gamma_\kappa)$	$-6\sqrt{3}XY$	$-6\sqrt{3}XZ$	$-6\sqrt{3}YZ$
q_3	$4Y(1+2\cos\gamma_1\cos\gamma_2)$	$-4Z(1+2\cos\gamma_1\cos\gamma_2)$	0	$-6\sqrt{3}XY$	$\mathcal{J}_3$	0	0
q_2	$-4Z(1+2\cos\gamma_1\cos\gamma_3)$	0	$+4X(1+2\cos\gamma_1\cos\gamma_3)$	$-6\sqrt{3}XZ$	0	$\mathcal{J}_2$	0
q_1	0	$4Z(1+2\cos\gamma_2\cos\gamma_3)$	$-4Y(1+2\cos\gamma_1\cos\gamma_3)$	$-6\sqrt{3}YZ$	0	0	$\mathcal{J}_1$

If we define

$$\rho^2 \equiv \sum_\nu |a_\nu|^2 = \sum_\kappa x_\kappa^2[1+4\cos^2\gamma_\kappa], \qquad (2.21)$$

the diagonal components of the inertia tensor can be written as

$$\mathcal{J}_\kappa = B\{4\rho^2 - 2\sqrt{21}\,\eta\cos\gamma_\kappa\}. \qquad (2.22)$$

C. Quantization of the Hamiltonian

The next problem is that of quantizing the Hamiltonian. There is no unique way to perform this quantification but, as in the quadrupole case [17], the Pauli prescription can be used. This recipe is designed to give the right answer when the generalized variables are transformed to Cartesian coordinates. Given a classical Hamiltonian written in terms of variables α_ν and their time derivatives, with a kinetic energy given by

$$\mathcal{T} = \frac{1}{2}\sum_{mn} G_{mn}(\alpha)\dot{\alpha}_m\dot{\alpha}_n, \qquad (2.23)$$

the Pauli prescription replaces the kinetic energy by the operator

$$\mathcal{T} = -\frac{1}{2}\sum_{mn} |G|^{-1/2}\frac{\partial}{\partial\alpha_m}|G|^{1/2}G^{mn}\frac{\partial}{\partial\alpha_n}, \qquad (2.24)$$

where $|G|$ is the determinant of the inertia matrix G_{mn} and G^{mn} is its inverse matrix. The volume element to be used is given by

$$d\tau = |G|^{1/2}\prod_n d\alpha_n. \qquad (2.25)$$

In our case, the variables are X,Y,Z,γ,q_1,q_2,q_3, and the inertia matrix G_{mn} is shown in Table I.

III. SYMMETRY PROPERTIES

A. General structure of the wave functions

The total collective Hamiltonian will contain a potential energy depending on the internal collective variables (and its time derivatives) in addition to the kinetic energy terms already discussed. The eigenfunctions of the total Hamiltonian can be labeled by the parity, the angular momentum and its projection on the laboratory z-axis (τ, I, and I_z). They can be conveniently expressed as a linear combination

$$\Psi^\tau_{I,I_z}(X,Y,Z,\gamma,\omega_i) = \sum_K g^\tau_{K,\xi}(X,Y,Z,\gamma)\mathcal{D}^\lambda_{I_z,K}(\omega_i), \qquad (3.1)$$

where the quantum numbers ξ, related to the internal variables, remain yet unspecified. This set of eigenfunctions constitute a complete set of states and they will be orthogonal using $d\tau$ specified in Eq. (2.25) as volume element.

B. Invariants and the potential energy in Bohr's Hamiltonian

As in the collective descriptions studied before [19,17,21], there are two types of symmetries that arise in the problem of collective motion. The first type corresponds to the invariance under rotations. The second type is related to the fact that even if the collective variables in the lab system are uniquely determined, there are 24 different ways of defining a right-handed intrinsic system [2]. For simplicity, it is commonly assumed that the potential energy does not depend on the velocities, and that it should be an analytic function when written in terms of the α_μ. Naturally, it must also be a scalar under rotations, and it is therefore important to search for simple polynomials in terms of the α_μ that are scalar under rotations. It is well known that in the quadrupole case there are two of the so-called basic invariants [17] (β^2 and $\beta^3 \cos 3\gamma$) while in the $T=1$ pairing case there are three basic scalars under rotations [Δ^2 and $\Delta^2 e^{\pm 4i\phi} \cos(2\Gamma)$], but only two if one requires invariance with regard to rotations both in usual space and in gauge space [Δ^2 and $\Delta^4 \cos^2(2\Gamma)$].

In the octupole case it is possible to find in a simple way some of these basic scalars with regard to rotations (we use the same notation as Kumar and Baranger [17]). The first one is quite trivial (the upper index denotes the number of bosons needed to construct the scalar):

$$I^{(2)} = \rho^2 = \sum_\mu \alpha_\mu^* \alpha_\mu = -\sqrt{7}\{aa\}_0^0. \qquad (3.2)$$

The second and third ones can be constructed in a similar way as in the quadrupole case using u_m, the quadrupole variables related to the inertia tensor, i.e.,

$$I^{(4)} = \{uu\}_0^0 = \frac{1}{\sqrt{5}} \eta^2, \qquad (3.3)$$

$$I^{(6)} = \{\{uu\}^2 u\}_0^0 = -\sqrt{\frac{2}{35}} \eta^3 \cos 3\gamma. \qquad (3.4)$$

To be sure that one has obtained all the basic scalars it is convenient to count the states with angular momentum zero and check that they can be constructed out of the elementary scalars already known. The number of states having angular momentum zero for each number of bosons can be constructed in a simple way using the m-scheme. Studying the states obtained considering up to 40 bosons it is found that it is necessary to introduce a basic scalar formed with ten bosons.[2] Its existence shows how much more complicated is the octupole case as compared with the other collective treatments already performed.

C. Wave function's symmetry properties

In this subsection we will follow closely Ref. [17]. The wave function Ψ must be an analytical function of the coor-

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[2] We would like thank to Professor J. Blomqvist who called our attention to the existence of this tenth order invariant.

dinates α_μ. The lab variables are unambiguously defined while, as Bohr already noted, the intrinsic variables a_m are not, as there are 24 ways of defining a right-handed intrinsic system starting from one lab system.

This can be seen more clearly if one defines three basic operators which can be used to transform a given intrinsic system in an equivalent one:

$\mathcal{R}_1$: rotation through π around the 1-axis of the intrinsic system.

$\mathcal{R}_2$: rotation through $\pi/2$ around the 3-axis of the intrinsic system.

$\mathcal{R}_3$: cyclic permutation of the three intrinsic axes.

Since $\mathcal{R}_1^2 = \mathcal{R}_2^4 = \mathcal{R}_3^3 = 1$, the 24 possible transformations between equivalent intrinsic systems are $\mathcal{S}(s_1,s_2,s_3) = \mathcal{R}_1^{s_1} \mathcal{R}_2^{s_2} \mathcal{R}_3^{s_3}$ with $0 \le s_1 \le 1$, $0 \le s_1 \le 3$, and $0 \le s_1 \le 2$. There are then 24 ways of choosing the a_m for a given α_μ, but Ψ must be the same for each of the choices, being invariant under the transformation that changes an intrinsic system to an equivalent one, i.e., Ψ must be invariant under any of the transformations $\mathcal{S}(s_1,s_2,s_3)$. All these transformations can be considered as acting on the coordinates $(X,Y,Z,\gamma,\theta,\phi,\psi)$. We have therefore that these transformations applied to a point:

$$\mathcal{R}_1(X,Y,Z,\gamma,\theta,\phi,\psi) = (X,Y,Z,\gamma,\pi-\theta,\phi+\pi,-\varphi),$$
$$\mathcal{R}_2(X,Y,Z,\gamma,\theta,\phi,\psi) = (X,Y,Z,\gamma,\theta,\phi,\varphi+\pi/2),$$
$$\mathcal{R}_3(X,Y,Z,\gamma,\theta,\phi,\psi) = (X,Y,Z,\gamma, \text{three new Euler angles}$$
$$\text{very complicated}).$$

These very complicated new Euler angles related to $\mathcal{R}_3$ correspond to the cyclic permutation of the axis but we will not need their explicit form.

In order to obtain the corresponding transformation R_k of wave functions Ψ we must apply the recipe for active transformations:

new wave function at new point

= old wave function at old point.

It is convenient to remember that the application of an active rotation R on a spherical tensor $\mathcal{T}_{lm}$ yields

$$[\mathcal{R}(\theta,\phi,\psi)\mathcal{T}]_{lm} = \sum_n \mathcal{D}_{m,n}^l(\theta,\phi,\psi)\mathcal{T}_{ln}. \qquad (3.5)$$

Writing the new wave function at the new point in terms of the old one at the old point one obtains

$$R|I,M\rangle = \sum_K \mathcal{D}_{M,K}^I(R^{-1})|I,K\rangle$$

$$= \sum_K [\mathcal{D}_{K,M}^I(\theta,\phi,\psi)]^*|I,K\rangle. \qquad (3.6)$$

A similar relation holds between a_m and α_μ, i.e., $a_m = \sum_\mu [\mathcal{D}_{m,\mu}^3(\theta,\phi,\psi)]^* \alpha_\mu$.

To obtain the effect of R_i on the $\mathcal{D}_{K,M}^I$ matrices it is convenient to relate R_i to the operator R_i' that performs the

TABLE II. Matrix elements of $\mathcal{D}^I_{M,K}(\pi/2,0,\pi/2)$.

$M\backslash K$	3	2	1	0	-1	-2	-3
3	$-\dfrac{i}{8}$	$-i\dfrac{\sqrt{6}}{8}$	$-i\dfrac{\sqrt{15}}{8}$	$-i\dfrac{\sqrt{20}}{8}$	$-i\dfrac{\sqrt{15}}{8}$	$-i\dfrac{\sqrt{6}}{8}$	$-\dfrac{i}{8}$
2	$\dfrac{\sqrt{6}}{8}$	$\dfrac{4}{8}$	$\dfrac{\sqrt{10}}{8}$	0	$-\dfrac{\sqrt{10}}{8}$	$-\dfrac{4}{8}$	$-\dfrac{\sqrt{6}}{8}$
1	$i\dfrac{\sqrt{15}}{8}$	$i\dfrac{\sqrt{10}}{8}$	$-\dfrac{i}{8}$	$-i\dfrac{\sqrt{12}}{8}$	$-\dfrac{i}{8}$	$i\dfrac{\sqrt{10}}{8}$	$i\dfrac{\sqrt{15}}{8}$
0	$-\dfrac{\sqrt{20}}{8}$	0	$\dfrac{\sqrt{12}}{8}$	0	$-\dfrac{\sqrt{12}}{8}$	0	$\dfrac{\sqrt{20}}{8}$
-1	$-i\dfrac{\sqrt{15}}{8}$	$i\dfrac{\sqrt{10}}{8}$	$\dfrac{i}{8}$	$-i\dfrac{\sqrt{12}}{8}$	$\dfrac{i}{8}$	$i\dfrac{\sqrt{10}}{8}$	$-i\dfrac{\sqrt{15}}{8}$
-2	$\dfrac{\sqrt{6}}{8}$	$-\dfrac{4}{8}$	$\dfrac{\sqrt{10}}{8}$	0	$-\dfrac{\sqrt{10}}{8}$	$\dfrac{4}{8}$	$-\dfrac{\sqrt{6}}{8}$
-3	$\dfrac{i}{8}$	$-i\dfrac{\sqrt{6}}{8}$	$i\dfrac{\sqrt{15}}{8}$	$-i\dfrac{\sqrt{20}}{8}$	$i\dfrac{\sqrt{15}}{8}$	$-i\dfrac{\sqrt{6}}{8}$	$\dfrac{i}{8}$

same transformation on the lab system, i.e., $R_i=RR'_iR^{-1}$, where R corresponds to the rotation (θ,ϕ,ψ). It is then possible to express

$$R_i\mathcal{D}^I_{M,N}(\theta,\phi,\psi)=RR'_iR^{-1}\mathcal{D}^I_{M,N}(\theta,\phi,\psi). \qquad (3.7)$$

Applying three times Eq. (3.6) on the right-hand side one gets

$$\sum_{KPQ}\mathcal{D}^I_{M,K}(R)\mathcal{D}^I_{K,P}(R'^{-1}_i)\mathcal{D}^I_{P,Q}(R^{-1})\mathcal{D}^I_{Q,N}(\theta,\phi,\psi)$$

$$=\sum_K\mathcal{D}^I_{M,K}(\theta,\phi,\psi)\mathcal{D}^I_{K,N}(R'^{-1}_i), \qquad (3.8)$$

where in the last step the unitarity of the $\mathcal{D}^I_{K,N}$ matrices was used.

Taking into account that the wave functions can be written as

$$\Psi^\tau_{I,M}(X,Y,Z,\gamma,\theta,\phi,\psi)=\sum_K g^\tau_{I,K}(X,Y,Z,\gamma)\mathcal{D}^\lambda_{M,K}(\theta,\phi,\psi), \qquad (3.9)$$

and taking into account that the symmetry of the wave function with regard to R_1, R_2, and R_3 implies that

$$R_i\Psi^\tau_{I,M}(X,Y,Z,\gamma,\theta,\phi,\psi)=\Psi^\tau_{I,M}(X,Y,Z,\gamma,\theta,\phi,\psi), \qquad (3.10)$$

and considering the effect of R_i on the intrinsic and rotational degrees of freedom

$$R_i\mathcal{D}^I_{M,K}(\theta,\phi,\psi)=\mathcal{D}^I_{M,K}(\theta',\phi',\psi')$$

$$=\sum_{K'}\mathcal{D}^I_{M,K'}(\theta,\phi,\psi)\mathcal{D}^I_{K',K}(R'^{-1}_i), \qquad (3.11)$$

$$R_ig^\tau_{I,K}(X,Y,Z,\gamma)=g^\tau_{I,K}(X',Y',Z',\gamma'), \qquad (3.12)$$

it is possible to obtain a condition on the part of the wave function that depends on the internal variables:

$$g^\tau_{I,K'}(X,Y,Z,\gamma)=\sum_K g^\tau_{I,K}(X',Y',Z',\gamma)\mathcal{D}^I_{K',K}(R'^{-1}_i). \qquad (3.13)$$

In order to obtain the effect of the symmetry operation on the internal variables, we must first evaluate $\mathcal{D}^I_{M,K}(R_i)$ explicitly. A lengthy yet straightforward calculation yields

$$\mathcal{D}^I_{M,K}(R_1)=(-1)^I\delta_{M,-K}, \qquad (3.14)$$

$$\mathcal{D}^I_{M,K}(R_2)=(-i)^K\delta_{M,K}, \qquad (3.15)$$

$$\mathcal{D}^I_{M,K}(R_3)=\mathcal{D}^I_{M,K}\left(\frac{\pi}{2},0,\frac{\pi}{2}\right). \qquad (3.16)$$

This last matrix is shown in Table II.

From the transformation properties of the coefficients a_m, one can deduce the transformation properties for X, Y, Z, and γ. In Table III we show all the information related to the transformation properties of the variables, as well as the characteristics of the matrices related with $\mathcal{D}^I_{K,K'}(R'^{-1}_i)$.

With regard to the spatial inversion $\mathcal{P}$, which is not a symmetry property due to ambiguities in the definition of the

TABLE III. Action of the different transformation operators on the corresponding intrinsic variables. Also shown are the explicit representation of $\mathcal{D}^I_{K,K'}(R_i^{-1})$.

Variable\Transformation	R_1	R_2	R_3
X'	X	$-Y$	Z
Y'	$-Y$	X	X
Z'	$-Z$	Z	Y
γ	γ	$-\gamma$	$\gamma + \dfrac{2\pi}{3}$
θ	$\pi - \theta$	θ	Complicated
ϕ	$\pi + \phi$	ϕ	Complicated
ψ	$-\psi$	$\psi + \dfrac{\pi}{2}$	Complicated
$\mathcal{D}^I_{K,K'}(R_i^{-1}).$	$(-1)^I \delta_{K,-K'}$	$(-i)^K \delta_{K,K'}$	$\mathcal{D}^I_{K,K'}\left(\dfrac{\pi}{2},\dfrac{\pi}{2},\pi\right)$

intrinsic axis, but must be a symmetry of the intrinsic wave function, one obtains $\mathcal{P}:(X,Y,Z,\gamma) \rightarrow (-X,-Y,-Z,\gamma)$ and $\mathcal{P}^I_{K,K'} = (-1)^I \delta_{K,K'}$, that replaces the $\mathcal{D}^I_{K,K'}$ in Eq. (3.13). The different transformations will then yield some symmetry properties of the wave function:

$$R_1 : g^\tau_{I,K}(X,Y,Z,\gamma) = (-1)^I g^\tau_{I,-K}(X,-Y,-Z,\gamma), \quad (3.17)$$

$$R_2 : g^\tau_{I,K}(X,Y,Z,\gamma) = (-i)^K g^\tau_{I,K}(-Y,X,Z,-\gamma), \quad (3.18)$$

$$R_3 : g^\tau_{I,K}(X,Y,Z,\gamma) = \sum_{K'} g^\tau_{I,K'}\left(X,Y,Z,\gamma + \frac{2\pi}{3}\right) \times \mathcal{D}^I_{K,K'}\left(\frac{\pi}{2},\frac{\pi}{2},\pi\right). \quad (3.19)$$

There are some combinations of these operators that yield more useful results, such as

$$R_2^2 : g^\tau_{I,K}(X,Y,Z,\gamma) = (-1)^K g^\tau_{I,K}(-X,-Y,Z,\gamma), \quad (3.20)$$

$$R_2^2 R_1 : g^\tau_{I,K'}(X,Y,Z,\gamma) = (-1)^{I+K} g^\tau_{I,-K}(-X,Y,-Z,\gamma). \quad (3.21)$$

If the wave function is also an eigenfunction of the parity operator with eigenvalue Π, i.e.,

$$\mathcal{P}\Psi^\tau_{I,M}(X,Y,Z,\gamma,\theta,\phi,\psi) = \Pi \Psi^\tau_{I,M}(X,Y,Z,\gamma,\theta,\phi,\psi), \quad (3.22)$$

we obtain that

$$\mathcal{P}: g^\tau_{I,K}(X,Y,Z,\gamma) = \Pi(-1)^I g^\tau_{I,K}(-X,-Y,-Z,\gamma). \quad (3.23)$$

IV. THE RIGID ROTOR

In this section we study the axially symmetric rotor. Axial symmetry implies that at least two of the diagonal components of the inertia tensor must be equal. From Eq. (2.22) it follows that for $\gamma=0$ or $\gamma=\pi/3$ this condition is satisfied. It is also possible to make the three components of the inertia tensor equal by making all the three x_k equal (in this particular case $\eta=0$). For $\gamma=0$ one has $\mathcal{J}_1=\mathcal{J}_2$ while for $\gamma=\pi/3$ one has $\mathcal{J}_1=\mathcal{J}_3$. In both cases the remaining component does not vanish. We will study in some detail the $\gamma=0$ case because it illustrates some of the complications and features related to the octupole degrees of freedom.

We will assume in this section that the γ degree of freedom is frozen (in particular γ is equal to zero). It follows also from the relation between the collective variables in the intrinsic system (a_μ) and the intrinsic variables (X, Y, Z, and γ) given by Eqs. (2.19) that $\gamma=0$ implies that the only deformations allowed should have $K=0$ or $K=\pm 3, \pm 6, \ldots$. It must be noted that when the collective description of the $T=1$ pairing excitations was studied in Refs. [21,23], it was found that for studying the rigid rotor it was necessary to retain the gauge angle degree of freedom as the rotational Hamiltonian was coupled to it. In this section, even if the rotational Hamiltonian is coupled to the γ degree of freedom we will assume that it is possible to freeze it and we will therefore disregard it completely. In this case the two basic quantities ρ^2 and β can be written as

$$\rho^2 = 2(X^2 + Y^2) + 5Z^2, \quad (4.1)$$

$$\beta = \frac{10}{\sqrt{21}}\left(-\frac{1}{2}(X^2 + Y^2) + Z^2\right), \quad (4.2)$$

and the inertia tensor has a rather simple expression in terms of the intrinsic variables:

$$\mathcal{J}_1 = \mathcal{J}_2 = 3(X^2 + Y^2) + 30Z^2,$$

$$\mathcal{J}_3 = 18(X^2 + Y^2). \quad (4.3)$$

TABLE IV. Inertia matrix G_{mn} for the $\gamma = 0$ case.

	$\dot{\rho}$	$\dot{\mu}$	$\dot{\zeta}$	q_1	q_2	q_3
$\dot{\rho}$	1	0	0	0	0	0
$\dot{\mu}$	0	ρ^2	0	0	0	0
$\dot{\zeta}$	0	0	$\rho^2 \sin^2 \mu$	$-3\rho^2 \sin^2 \mu$	0	0
q_1	0	0	$-3\rho^2 \sin^2 \mu$	$9\rho^2 \sin^2 \mu$	0	0
q_2	0	0	0	0	$6\rho^2[1 - \frac{3}{4} \sin^2 \mu]$	0
q_3	0	0	0	0	0	$6\rho^2[1 - \frac{3}{4} \sin^2 \mu]$

It is convenient to reparametrize the problem in order to introduce ρ as one of the dynamical variables and use ''spherical coordinates'' by defining two angle variables μ and ζ

$$X = \rho \sin \mu \cos \zeta / \sqrt{2},$$

$$Y = \rho \sin \mu \sin \zeta / \sqrt{2},$$

$$Z = \rho \cos \mu / \sqrt{5}. \tag{4.4}$$

In terms of these variables $\beta = (10/\sqrt{21})\rho^2[-\frac{1}{4} \sin^2 \mu + \frac{1}{5} \cos^2 \mu]$. Now the G_{mn} inertia matrix will be a six by six matrix as shown in Table IV.

We will assume the adiabatic hypothesis for ρ and μ. But it must be noted that, as ζ is a cyclic coordinate, we cannot use for it the adiabatic hypothesis and we must, therefore, consider the coupling of $\dot{\zeta}$ with q_1, q_2, and q_3 in an exact way. For this purpose we use the conjugate momentum method, i.e., we introduce

$$Q_1 = \frac{\partial \mathcal{T}}{\partial q_1} = 6\rho^2\left[1 - \frac{3}{4} \sin^2 \mu\right] q_1, \tag{4.5}$$

$$Q_2 = \frac{\partial \mathcal{T}}{\partial q_2} = 6\rho^2\left[1 - \frac{3}{4} \sin^2 \mu\right] q_2, \tag{4.6}$$

$$Q_3 = \frac{\partial \mathcal{T}}{\partial q_3} = 9\rho^2 \sin^2 \mu\left[q_3 - \frac{1}{3}\dot{\zeta}\right] = K, \tag{4.7}$$

$$P_\zeta = \frac{\partial \mathcal{T}}{\partial \dot{\zeta}} = -3\rho^2 \sin^2 \mu\left[q_3 - \frac{1}{3}\dot{\zeta}\right] = -i\frac{\partial}{\partial \zeta} = m_\zeta. \tag{4.8}$$

It must be noted that Q_i satisfy the commutation relations given by Eqs. (2.8). Besides, the relation between Eq. (4.7) and Eq. (4.8) provides the auxiliary condition:

$$K = -3m_\zeta = 0, \pm 3, \pm 6, \dots . \tag{4.9}$$

The kinetic energy can be written in terms of these new variables Q_κ as

$$\mathcal{T}_{\text{rot}} = \sum_\kappa \frac{1}{2\mathcal{J}_\kappa} Q_\kappa^2, \tag{4.10}$$

where the components of the moment of inertia are given by

$$\mathcal{J}_1 = \mathcal{J}_2 = \frac{3}{4}\rho^2[1 + 3\cos^2 \mu],$$

$$\mathcal{J}_3 = \frac{9}{2}\rho^2 \sin^2 \mu. \tag{4.11}$$

The total rotational energy can be written as

$$\mathcal{T}_{\text{rot}} = \frac{I(I+1)}{2\mathcal{J}_1} + \frac{K^2(\mathcal{J}_1 - \mathcal{J}_3)}{2\mathcal{J}_1 \mathcal{J}_3}$$

$$= \frac{\left[I(I+1) + \frac{2}{3} K^2 \dfrac{\left[1 - \frac{9}{4} \sin^2 \mu\right]}{\sin^2 \mu}\right]}{2\mathcal{J}_1}. \tag{4.12}$$

The structure of the full ''rotational band'' is now more complicated than for the quadrupole case. The part of the band that has $K=0$ has a structure similar to that of the usual rigid quadrupole band, but the part of the band related to the states with $K \neq 0$ has energies determined also by ρ and μ that are related with the energy of the first member of the ground state rotational band. Note that μ represents deviations from perfectly axisymmetric deformations, i.e., for $\mu = 0$ the deformations have $\mathcal{J}_3 = 0$ and therefore $K \equiv 0$, only for $\mu \neq 0$ can nonzero K be found. For $\mu = 0$ the rotational band has the usual structure (all states have $K = 0$, as states with $K \neq 0$ have an infinite energy). When the states with angular momentum equal or larger than 3 are considered it is found that there are more than one state belonging to the ground state band with this angular momentum: one with $K=0$ and parity $(-1)^I$, and two with $K=3$ and energies given by Eq. (4.12). Each time that $I = |K| = 3n$ (with n integer) two new states appear (i.e., we will have five states with $8 \geq I \geq 6$, seven states with $11 \geq I \geq 9$, etc.). Figure 1 shows the lowest energy states for $K = 0, 3, 6$ as a function of μ.

V. SUMMARY

In the present paper we have obtained a parametrization of the octupole collective variables that guarantees that the inertia tensor is diagonal. The relation between the components of the octupole intrinsic variables and those defined parameters is given by the equations
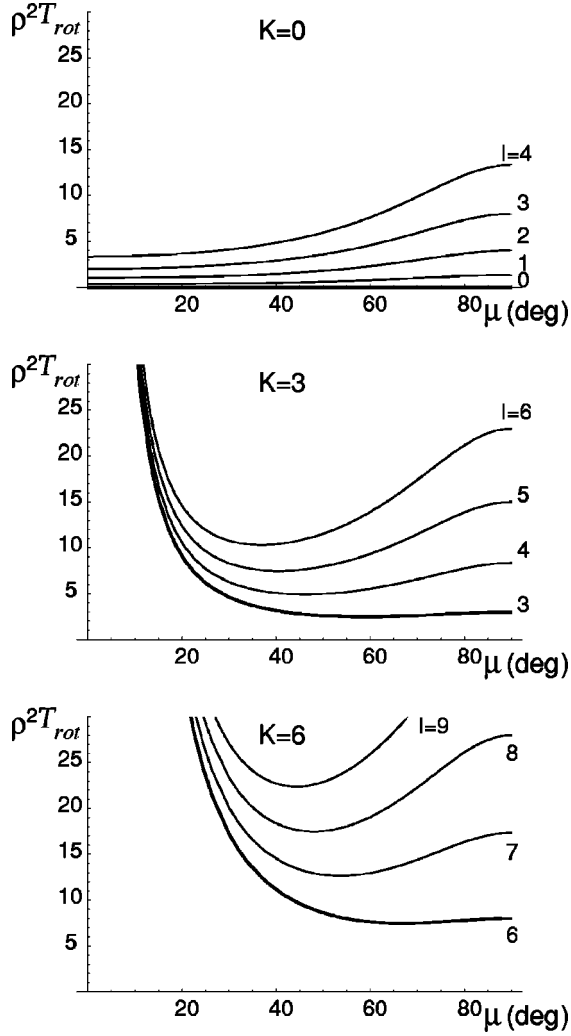
The first condition means that the parameters X, Y, and Z can be considered as positive, as all the other signs can be obtained by relabeling the axis. The second statement, as in the quadrupole case, tells us that all possible shapes are contained in the range $0 \leq \gamma \leq \pi/3$.

A general octupole field can be written in an alternative way [16] as $V_3 = \Sigma_m a_m Y_{3m}^* = \epsilon_0 A_2 + \Sigma_{i=1}^3 \epsilon_1(i) F_1(i) + \Sigma_{i=1}^3 \epsilon_2(i) F_2(i)$, where A_1, $F_1(k)$, and $F_2(k)$ are related to the irreducible representations of the octahedron group. In Ref. [16] it was proposed that an appropriate parametrization can be obtained imposing the cancelation of $\epsilon_2(i) \forall i$. Using the parametrization that we are proposing, these parameters have now a rather simple structure:

$$\epsilon_0 = 0,$$

$$\epsilon_1(1) = -\sin(\gamma)Z,$$

$$\epsilon_1(2) = -\sin\left(\gamma - \frac{2\pi}{3}\right)X,$$

$$\epsilon_1(3) = \sin\left(\gamma - \frac{4\pi}{3}\right)Y,$$

$$\epsilon_2(1) = \sqrt{5}\cos(\gamma)Z,$$

$$\epsilon_2(2) = \sqrt{5}\cos\left(\gamma - \frac{2\pi}{3}\right)X,$$

$$\epsilon_2(2) = -\sqrt{5}\cos\left(\gamma\frac{4\pi}{3}\right)Y.$$

It must be noted that, for the octupole degrees of freedom, the existence of axial symmetry does not necessarily imply that the rotational band must have $K=0$. The study of the rigid rotor has illustrated the richness of the octupole rotational bands.

Last but not least, it is worthwhile noticing that if one takes into account simultaneously the quadrupole and octupole degrees of freedom, and for each one of them the condition that the inertia tensor has to be diagonal is imposed, the intrinsic system for both degrees of freedom will not be the same: each degree of freedom will have its own "intrinsic system." It must be remembered that the Euler angles associated to each intrinsic system are just a way of labeling three of the five (in the quadrupole case) or seven (in the octupole one) collective dynamical variables.

FIG. 1. Spectrum of a symmetric ($\gamma=0$) rigid rotor for $K = 0, 3, 6$ as a function of the deformation parameter μ.

$$a_3 = \left[\cos\gamma - \frac{\sqrt{3}}{2}\sin\gamma\right]X + i\left[\cos\gamma + \frac{\sqrt{3}}{2}\sin\gamma\right]Y,$$

$$a_2 = \frac{1}{\sqrt{2}}\sin\gamma Z,$$

$$a_1 = \frac{\sqrt{5}}{2}\sin\gamma[X+iY],$$

$$a_0 = \sqrt{5}\cos\gamma Z.$$

In addition, we have identified the way in which the intrinsic variables (x_k and γ) transform with regard to the symmetry operations R_i. These can be summarized as follows: (a) The variables x_k transform in a similar way as the coordinates of a vector related to the intrinsic axis; (b) γ transforms in the same way as in the quadrupole case. This is not at all strange due to the particular relation of γ to the inertia tensor.

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