Chapter 1

The octupole collective Hamiltonian.
Does it follow the example of the quadrupole case?

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A general form of the octupole collective Hamiltonian is introduced and analyzed based on fundamental tensors in the seven-dimensional tensor space. Possible definitions of intrinsic frames of reference possessing cubic symmetry for the octupole tensor are considered. Cubic intrinsic octupole coordinates or deformations are introduced. Shapes of the octupoloid are investigated. The octupole collective Hamiltonian is expressed in intrinsic coordinates. An intrinsic angular momentum carried by the octupole vibrations is discovered. Small oscillations about an axially-symmetric pear shape are analyzed. Formulation of a unified quadrupole-octupole collective model is discussed.

1. Introduction

The idea of attributing a definite multipolarity to nuclear collective excitations came from the nuclear liquid-drop model. It was known before the discovery of atomic nuclei that the normal modes of the surface vibrations of a spherical drop of incompressible liquid have definite multiplicities. Many years later, when atomic nuclei were already known, Siegfried Flügge connected the eigenfrequencies of the surface vibrations of a nuclear liquid drop with the excitation energies of low-lying states of even-even nuclei. These were the beginnings of the collective model.

The most important collective mode in nuclear structure physics is that with multipolarity \( \lambda = 2 \), because it concerns the lowest excited states in even-even nuclei. These states are well known experimentally and theoretical methods describing them are well developed. One such method, applicable to even-even nuclei only, is a
description by means of the Schrödinger equation in a collective space. Initiated by Aage Bohr [3] a long time ago, it is very effective and is still in use. The Bohr Hamiltonian became the label of the model. When applying the method one usually starts with a general classical collective Hamiltonian [4, 5]. Its form has been extracted from various microscopic many-body models through methods of the “Adiabatic Time-Dependent Hartree-Fock-Bogolyubov” (ATDHFB) type (see e.g. Chapt. 12 in Ref. [6]) and then quantized by means of the Podolsky-Pauli prescription [7–9]. Such a quasi-classical approach is still used even today. It would be good to use purely quantum methods to describe the collective states. Therefore, the Generator Coordinate Method (GCM) has been recently employed [10, 11]. It leads to integral equations instead of differential ones (see e.g. Chapt. 10 in Ref. [6]). However, in an approximation to the GCM called the Gaussian Overlap Approximation (GOA) the Hill-Wheeler integral equations for collective motion can be reduced back to differential equations with a collective Hamiltonian [12].

Apart from the positive-parity quadrupole states, negative-parity levels have been observed for a long time [13] in the low-energy spectra of even-even nuclei. Multipolarity $\lambda = 3$ has been attributed to such states. Information on the octupole states has been collected over many years, see Refs. [14] and [15] for reviews. Recently, measurements of a static octupole deformation in radium ($^{224}$Ra) and barium ($^{144}$Ba) isotopes have been reported [16, 17]. However, data on the octupole states are not so rich as in the case of quadrupole excitations. This is perhaps connected with experimental and interpretational difficulties. A common opinion seems to be that the quadrupole collective Hamiltonian stands for a pattern for higher multipoles. However, it is not so easy. The theory of the octupole degrees of freedom is much more complicated than that of the quadrupole ones, or rather the quadrupole case is exceptionally simple. This will be demonstrated further in subsequent Sections. In Sec. 2 a general form of the octupole collective Hamiltonian is introduced and discussed in comparison with that of the quadrupole one. Possible definitions of intrinsic frames of reference for the octupole tensor in analogy to that for the quadrupole tensor are considered in Sec. 3.1. The octupole deformation parameters are introduced and illustrated. The octupole Hamiltonian is expressed in intrinsic coordinates in Sec. 3.2. Its approximate form for small oscillations around a pear shape is given in Sec. 3.3. In Conclusion, in Sec. 4 a draft of a unified quadrupole-octupole collective model is recapitulated.

2. General form of collective Hamiltonians

The idea of collective models consists generally in describing some complex (collective) states of a many-body system through the substitution of the coordinates of many particles by a relatively small number of collective variables. An appropriate choice of these collective variables decides the success of the model. Constructing the collective models in question here for the description of low-lying collective states of even-even nuclei one takes the spherical tensors $\alpha_\lambda$ as collective variables.
These tensors are transformed according to irreducible \((2\lambda + 1)\)-dimensional representations \(D^\lambda\) of the \(O(3)\) group of orthogonal transformations in the physical space. The spherical components \(\alpha_{\lambda\mu} (\mu = -\lambda, \ldots, \lambda)\) of \(\alpha_\lambda\) in the laboratory frame, \(U_{lab}\), are the collective laboratory coordinates. It is assumed that the tensor \(\alpha_\lambda\) is electric i.e. has parity \((-1)^\lambda\) and real, which means that its components fulfill the relation \(\alpha^*_\lambda\mu = (-1)^\mu \alpha_{\lambda-\mu}\). The differential operators \([-i\partial/\partial \alpha^*_\lambda\mu]\) play the role of the momenta canonically conjugate to the coordinates \(\alpha_{\lambda\mu}\). The angular momentum operators or the \(O(3)\) generators in the collective space fulfill characteristic commutation relations with the coordinates and momenta (see e.g. Appendix A.1. in Ref. \[18\]). The following vector operator:

\[
L^{(3)}_{\mu\nu}(\alpha_\lambda) = (-1)^\lambda \sqrt{\frac{\lambda(\lambda + 1)(2\lambda + 1)}{3}} \sum_{\kappa\nu}(\lambda\kappa\lambda\nu|1\mu)\alpha_{\lambda\kappa}\frac{\partial}{\partial \alpha^*_{\lambda\nu}}
\]

fulfills such commutation relations and thus plays the role of the collective angular momentum \[18, 19\].

The nuclear collective system is defined by a collective Hamiltonian \(H_\lambda(\alpha_\lambda)\). It is assumed that \(H_\lambda(\alpha_\lambda)\) has the following properties:

1. It is a second-order differential operator (like the Schrödinger operator),
2. it is real, i.e. \(H_\lambda(\alpha_\lambda) = H^*_\lambda(\alpha_\lambda)\) (it describes even-even nuclei only),
3. it is a scalar with respect to the orthogonal group \(O(3)\) (rotations and inversion in the physical space) or commutes with the angular momentum operators of Eq. \[1\],
4. it is Hermitian with a scalar weight \(W(\alpha_\lambda) \geq 0\),
5. it possesses the lowest eigenvalue (positive kinetic energy),
6. it is an isotropic function of the coordinates, i.e. it does not depend on any other tensor quantities.

No other assumptions are needed at this stage (cf. Ref. \[20\]). The most general form of \(H_\lambda(\alpha_\lambda)\) with properties (1) – (6) given above reads \[12, 18\]:

\[
H_\lambda(\alpha_\lambda) = -\frac{1}{2W(\alpha_\lambda)} \sum_{\mu,\nu} \frac{\partial}{\partial \alpha_{\lambda\mu}} W(\alpha_\lambda) B^{-1}_{\lambda\mu\lambda\nu}(\alpha_\lambda) \frac{\partial}{\partial \alpha^*_{\lambda\nu}} + V(\alpha_\lambda),
\]

The Hamiltonian is determined by three quantities: two real scalar functions — weight \(W(\alpha_\lambda)\) and potential \(V(\alpha_\lambda)\), and a symmetric \((2\lambda + 1) \times (2\lambda + 1)\) matrix of real so-called inverse inertial functions \(B^{-1}_{\lambda\mu\lambda\nu}(\alpha_\lambda)\). Since the matrix is transformed under the \(O(3)\) group like a product of two tensors \(\alpha_\lambda\) it is called a symmetric bitensor. All these three quantities depend on no other tensors but \(\alpha_\lambda\) and therefore they are isotropic tensor fields in the \((2\lambda + 1)\)-dimensional collective space. They can either be calculated from microscopic many-body models or fitted to experimental data. When the Hamiltonian is obtained by quantization of its classical counterpart the weight is \(W(\alpha_\lambda) = \sqrt{\text{det} B_{\lambda\mu\lambda\nu}(\alpha_\lambda)}\).

\[\text{Units } \hbar = c = 1 \text{ are used here.}\]
In order to investigate possible structures of the inverse inertial bitensor it is convenient to express it as a set of (single) tensors $T_{2l}(\alpha_\lambda)$ ($l = 0, \ldots, \lambda$), namely

$$B_{\lambda \mu \lambda \nu}(\alpha_\lambda) = \sum_{l=0}^{\lambda} (\lambda \mu \lambda \nu | 2l m) T_{2l} m(\alpha_\lambda)$$  \hspace{1cm} (3)

Assumption (6), that the $T_{2l}(\alpha_\lambda)$ are isotropic functions of $\alpha_\lambda$ is essential here.

Then, an arbitrary tensor $T_\Lambda(\alpha_\lambda)$ can be expressed in the following form:

$$T_\Lambda(\alpha_\lambda) = \sum_{k=1}^{k_{\lambda \Lambda}} \sigma_\Lambda^{(\Lambda)}(\alpha_\lambda) \tau_k \Lambda(\alpha_\lambda)$$  \hspace{1cm} (4)

by a number of definite fundamental tensors $\tau_k \Lambda(\alpha_\lambda)$ for given $\lambda$ and $\Lambda$, and arbitrary scalar coefficients $\sigma_\Lambda^{(\Lambda)}(\alpha_\lambda)$ (see Appendix A in Ref. [18]). The original Bohr inverse inertial bitensor [3] has the following form:

$$B_{\lambda \mu \lambda \nu}(\alpha_\lambda) = (\lambda \mu \lambda \nu | 00)(-1)^{\lambda} \sqrt{2\lambda + 1} \frac{1}{B_\lambda} = \frac{(-1)^{\mu} \delta_{\mu \nu}}{B_\lambda}$$  \hspace{1cm} (5)

where $B_\lambda$ is a constant mass parameter.

In the case of a general quadrupole ($\lambda = 2$) collective Hamiltonian it is well known that the inverse inertial bitensor can have at most six independent components out of fifteen possible ones [5, 18]. It is interesting to know whether there are similar restrictions for the components of the inverse inertial bitensor in the case of an octupole ($\lambda = 3$) collective Hamiltonian. Unfortunately, the things are much more complicated in that case. The symmetric bitensor $B_{\lambda \mu \lambda \nu}(\alpha_3)$ has twenty-eight components. Can they all be independent? To answer this question one should analyze Eqs. (3) and (4) for $\lambda = 3$.

According to Eq. (3) the even (positive-parity) symmetric octupole bitensor, $B_{\lambda \mu \lambda \nu}(\alpha_3)$, can be replaced with four tensors $T_{2l}(\alpha_3)$ ($l = 0, \ldots, 3$). These tensors should be even isotropic functions of $\alpha_3$. The tensor fields in the space of the octupole coordinates are built out of some twenty-six elementary tensors

$$t^{(\mu \nu)}_l = [\alpha_3 \times \ldots \times \alpha_3]_l$$

(square brackets $[\ldots]$ stand for vector coupling to rank $l$) for $l < 3n$ and related to each other by about two hundred syzygies or relations in the form of rational integral functions [21]. All the elementary tensors split into two groups with positive and negative spin-parity $(-1)^{l+n}$, respectively. Independent fundamental tensors $\tau_k \Lambda(\alpha_3)$ from Eq. (4) are constructed by alignment of the elementary tensors of Eq. (6). The positive spin-parity elementary and even (positive parity) fundamental tensors needed to construct the inverse inertial bitensor in question are listed in Sec. A.1. There are twenty-eight relevant fundamental tensors altogether and thus, all twenty-eight components of the bitensor $B_{\lambda \mu \lambda \nu}(\alpha_3)$ can be arbitrary tensor fields in the octupole collective space. No additional relations between the components need appear. Twenty-eight scalars $\sigma_\Lambda^{(\Lambda)}(\alpha_3)$ for $k = 1, \ldots, k_{3\Lambda}$ and $\Lambda = 0, 2, 4, 6$ are functions of the four elementary scalars, Eq. (A.1).
3. Intrinsic frame and intrinsic coordinates

3.1. Intrinsic frames of reference

Obviously, the tensor \( \alpha_{\lambda} \) can be represented by different sets of coordinates in different frames of reference. As already stated in Sec. 3, the \( \alpha_{\lambda\mu} \) are the components of \( \alpha_{\lambda} \) in the frame \( U_{\text{lab}} \). Let us take another frame, say \( U_{\text{in}} \), the orientation of which with respect to the laboratory frame \( U_{\text{lab}} \) is given by the Euler angles \( \omega = (\varphi, \vartheta, \psi) \). We will not use the spherical components of \( \alpha_{\lambda} \) in the frame \( U_{\text{in}} \). Instead, we shall use their real and imaginary parts, \( a_{\lambda k} \) and \( b_{\lambda k} \), respectively, defined in the standard way (cf e.g. Eq. A.7 in Ref. [18]). Then, the transformation rule between the corresponding components of the tensor \( \alpha_{\lambda} \) with respect to \( U_{\text{lab}} \) and \( U_{\text{in}} \), respectively, takes the following form (cf. Ref. [19]):

\[
\alpha_{\lambda\mu} = D_{\mu 0}^{\lambda}(\omega) a_{\lambda 0} + \sum_{k=1,2,3} \left[ D_{\mu k}^{\lambda}(\omega) a_{\lambda k} + D_{\mu k}^{\lambda -}(\omega) b_{\lambda k} \right]
\]

where

\[
D_{\mu k}^{\lambda}(\omega) = \frac{1}{\sqrt{2(1 + \delta_{k0})}} [D_{\mu k}^{\lambda}(\omega) + (-1)^k D_{\mu -k}^{\lambda}(\omega)]
\]

\[
D_{\mu k}^{\lambda -}(\omega) = \frac{i}{\sqrt{2}} [D_{\mu k}^{\lambda}(\omega) - (-1)^k D_{\mu -k}^{\lambda}(\omega)]
\]

are the semi-Cartesian Wigner functions. The Bohr-Mottelson definition of the Wigner functions, \( D_{\mu k}^{\lambda}(\omega) \), is used [22].

For the frame \( U_{\text{in}} \) to be the intrinsic frame, three properly chosen conditions for the coordinates \( a_{\lambda k} \) and \( b_{\lambda k} \) should be given, namely

\[
\Omega_i(a_{\lambda k}(\omega, \alpha_{\lambda\mu}), b_{\lambda k}(\omega, \alpha_{\lambda\mu})) = \Omega_i(\omega, \alpha_{\lambda\mu}) = 0
\]

for \( i = 1, 2, 3 \), which determine the three Euler angles, \( \omega = (\varphi, \vartheta, \psi) \) as functions of the laboratory coordinates and, in this way, impart the status of intrinsic coordinates to them. The remaining 2\( \lambda \) - 2 independent coordinates are usually called deformations.

The concept of an intrinsic (body-fixed) frame of reference is connected with the descriptions of collective states from the very beginning [3]. The principal axes of the tensor \( \alpha_{\lambda} \) are taken as the intrinsic axes in the quadrupole, \( \lambda = 2 \), case. According to Eq. (B.1) from Appendix B.2 the well-known definition of the intrinsic frame is \( g_{2s} = 0 \) for \( s = x, y, z \). It is seen from Appendix [3] that the frame \( U_{\text{in}} \) is then \( O_h \)-symmetric. The two remaining intrinsic coordinates, \( a_{20} = \beta \cos \gamma \) and \( a_{22} = \beta \sin \gamma \), are usually parametrized by the well-known deformation parameters \( \beta \) and \( \gamma \).

The problem of the intrinsic frame for the octupole tensor, \( \alpha_{3} \), has appeared to be less transparent than that for \( \lambda = 2 \). The tensor has no principal axes and thus no obvious intrinsic frame. Early attempts to define an intrinsic frame failed (cf Ref. [23]). This was, perhaps, the reason why the intrinsic frame of reference was for a long time determined with the quadrupole tensor and octupole coordinates.
were treated as intrinsic coordinates with respect to that frame (cf. Ref. [19]). And what shall we do when any quadrupole tensor is not at our disposal?

In order to define an intrinsic frame for \( \lambda = 3 \), having the natural symmetry \( O_h \), it is convenient to decompose the tensor representation \( D_3 \) of the \( O(3) \) group onto the \( O_h \) irreps \( A_{-2} \), \( F_{-1} \) and \( F_{-2} \), respectively (see Appendix B.1). The corresponding representations will be called the octupole cubic Wigner functions \( A_{\mu}(\omega) \), \( F_{\mu s}(\omega) \), \( (s = x, y, z) \) and \( G_{\mu s}(\omega) \), \( (s = x, y, z) \), respectively. They are the following combinations of the semi-Cartesian Wigner functions:

\[
A_{\mu}(\omega) = D_{\mu 2}^{3(-)}(\omega) \\
F_{\mu x}(\omega) = \sqrt{\frac{3}{8}} D_{\mu 1}^{3(+)}(\omega) - \sqrt{\frac{5}{8}} D_{\mu 3}^{3(+)}(\omega), \\
F_{\mu y}(\omega) = \sqrt{\frac{3}{8}} D_{\mu 1}^{3(-)}(\omega) + \sqrt{\frac{5}{8}} D_{\mu 3}^{3(-)}(\omega), \\
F_{\mu z}(\omega) = D_{\mu 0}^{3(0)}(\omega) \\
G_{\mu x}(\omega) = \sqrt{\frac{5}{8}} D_{\mu 1}^{3(+)}(\omega) - \sqrt{\frac{3}{8}} D_{\mu 3}^{3(+)}(\omega) \\
G_{\mu y}(\omega) = -\sqrt{\frac{5}{8}} D_{\mu 1}^{3(-)}(\omega) + \sqrt{\frac{3}{8}} D_{\mu 3}^{3(-)}(\omega) \\
G_{\mu z}(\omega) = D_{\mu 2}^{3(-)}(\omega).
\]

(10)

The cubic Wigner functions form a unitary set. When using them the transformation rule of Eq. (7) takes the following form:

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

(11)

where \( b, f_s \) and \( g_s \) are the octupole cubic coordinates in the frame \( U_{in} \), proposed in Ref. [24] and defined in Appendix B.2.

It is seen that we have two possible definitions of the \( O_h \)-symmetric frame of reference. We can take Eq. (9) in the two following alternative forms: either \( g_s = 0 \) or \( f_s = 0 \) for \( s = x, y, z \). Here, we shall explore the former definition. Both of them are briefly discussed in Ref. [25]. We see from Eq. (11) that in the former case the following relation between the spherical laboratory coordinates and the Euler angles and the octupole deformations holds:

\[
\alpha_{3\mu}(\omega, b, f) = A_{\mu}(\omega)b + \sum_{s=x,y,z} F_{\mu s}(\omega)f_s
\]

(12)

The Jacobian of the transformation \( \alpha_{3\mu} \rightarrow \omega, b, f_s \) is equal to

\[
D_f(\vartheta, b, f_x, f_y, f_z) = 8\sin \vartheta \left[ b \left( b^2 - \frac{15}{16} (f_x^2 + f_y^2 + f_z^2) \right) + \frac{15}{8} \sqrt{\frac{15}{16}} f_x f_y f_z \right] \\
= 8\sin \vartheta d_f(b, f_s)
\]

(13)

The transformation (12) is reversible for the deformations contained aside from the hyper-surface \( D_f(\vartheta, b, f_x, f_y, f_z) = 0 \), where ambiguities appear arising from the
symmetries of the shape. The $F^1_\lambda$-covariant (vector) deformations $(f_x, f_y, f_z)$ are transformed under the $O_h$ transformations of the intrinsic frame like the Cartesian coordinates $x, y, z$ of a position vector. It follows directly from the $O_h$ symmetry that it is sufficient to consider, for instance, the region $0 \leq f_x \leq f_y \leq f_z$ of vector deformations forming an infinite triangular pyramid in three-dimensional space (see Fig. 1). The forty-eight pyramids obtained by all the $O_h$ transformations fill up the entire space. Deformation $b$ supplements the space of vector deformations to the four-dimensional space. It is invariant under rotations $R_1$ and $R_3$ and changes sign under $R_2$ and inversion $P$ together with the corresponding transformations of the vector deformations. Therefore, there are no additional restrictions on values of $b$ (see Fig. 4 below). The case when $f_x^2 + f_y^2 + f_z^2 = 0$ is an exception: it is sufficient then to consider values $b \geq 0$.

To learn the geometrical meaning of the deformation parameters, $b$ and $f_s$, one can investigate the shapes of the “octupoloid” given by the following equation in the spherical coordinates $R, \theta, \phi$:

$$ R(\theta, \phi) = R_0 \left[ 1 - A_0(\phi, \theta, 0) b + \sum_{s=x,y,z} (1 - 2 \delta_{s, 0}^2) F_{0s}(\phi, \theta, 0) f_s \right] $$

(14)

in accordance with the approach of Ref. [20], bearing in mind that $D^\lambda_{\mu \lambda}(\phi, \theta, 0) = (-1)^\mu \sqrt{4\pi/(2\lambda + 1)} Y_{\lambda\mu}(\theta, \phi)$. The shape of the octupoloid is defined by the set of deformations $b, f_x, f_y$ and $f_z$ up to the cubic group of transformations i.e. the Bohr rotations and mirror reflections (see Appendix B.1). Two octupoloids with identical axial-symmetric (pear) shapes but oriented differently are shown in Fig. 2. Obviously, the two sets of vector deformations then lie inside different pyramids of Fig. 1. Changing the sign of the deformation gives inverted octupoloids with the same shape as that in the figure. Examples of octupoloids with asymmetric shapes
are shown in Fig. 3. Their orientations and/or handedness can be changed by cubic group transformations of the deformations. For instance, changing the signs of all the deformations gives inverted octupoloids. However, when deformations belonging to one out of the two irreducible representations of the cubic group are transformed the shape of the octupoloid is changed, as shown in Fig. 4. Changing the sign of $b$ without changing the vector deformations gives a change of shape.
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(a) $f_z = 0.5, b = 0.5, f_x = f_y = 0$
(b) $f_z = 0.5, b = -0.5, f_x = f_y = 0$

Fig. 4. Two octupoloïds with opposite signs of deformation $b$ having different shapes.

3.2. The Hamiltonian in intrinsic coordinates

A reversible transformation between the laboratory and intrinsic coordinates allows us to use interchangeably one or another set of variables. The use of intrinsic coordinates is usually more convenient because it gives the possibility to separate variables, especially the Euler angles. It is evident for potentials depending on the laboratory coordinates through the elementary scalars, the number of which coincides with the number of deformations. Hence, the potential in Eq. (2) is a function of the number of deformation parameters characteristic for a given multipolarity: two for $\lambda = 2$ and four for $\lambda = 3$.

To express the kinetic part of the Hamiltonian and angular momenta in intrinsic coordinates we have to convert derivatives with respect to the laboratory coordinates into derivatives with respect to the intrinsic variables. As might be expected (cf. Ref. [27]), independently of the multipolarity of the collective space the components of the angular momentum of Eq. (1) can be expressed as

$$ L_{1\kappa}^{(N)} = D_{\kappa 0}^{(1+)}(\omega)L_z(\omega) - D_{\kappa 1}^{(1+)}(\omega)L_y(\omega) + D_{\kappa 1}^{(1-)}(\omega)L_y(\omega) $$

where $L_x, L_y, L_z$ are the Cartesian components of the intrinsic angular momentum depending on the Euler angles and their derivatives only and are given by the following standard formulae: (cf. e.g. Eq. (2.15) in Ref. [18]).

$$ L_x(\varphi, \vartheta, \psi) = -i \left( \frac{\cos \psi}{\sin \vartheta} \frac{\partial}{\partial \varphi} + \sin \psi \frac{\partial}{\partial \vartheta} + \cot \vartheta \cos \psi \frac{\partial}{\partial \psi} \right) $$

$$ L_y(\varphi, \vartheta, \psi) = -i \left( \frac{\sin \psi}{\sin \vartheta} \frac{\partial}{\partial \varphi} + \cos \psi \frac{\partial}{\partial \vartheta} - \cot \vartheta \sin \psi \frac{\partial}{\partial \psi} \right) $$

$$ L_z(\varphi, \vartheta, \psi) = -i \frac{\partial}{\partial \psi} $$
For $\lambda = 2$ the procedure for converting the derivatives is well known and is presented in detail, e.g., in Ref. [18]. A general quadrupole Hamiltonian expressed in intrinsic variables is divided into the vibrational part depending only on two deformations and the rotational Hamiltonian which contains the angular momenta $L_x$, $L_y$, $L_z$ and the deformation dependent moments of inertia. The intrinsic axes are always the principal axes of the tensor of inertia. When we take the kinetic energy with the Bohr inverted inertial bitensor the structure of the Hamiltonian will not change much. Namely, the mixed term in the vibrational kinetic energy will vanish and the remaining five kinetic-energy terms — vibrational and rotational — contain one common constant mass parameter $B_2$ instead of different deformation-dependent inertial functions.

The procedure for transforming the octupole collective Hamiltonian to intrinsic coordinates is more involved than that for the case of $\lambda = 2$. The first step of the procedure is conversion of the derivatives with respect to the laboratory coordinates into those with respect to the intrinsic variables. To do this one should calculate the derivatives of the intrinsic with respect to the laboratory coordinates. The transformation the reverse of that of Eq. (12) can be presented in the following entangled form:

$$
\begin{align*}
    b &= \sum_{\mu} (A_\mu(\omega))^* \alpha_{3\mu}, \\
    f_s &= \sum_{\mu} (F_{\mu s}(\omega))^* \alpha_{3\mu}, \\
    0 &= \sum_{\mu} (G_{\mu s}(\omega))^* \alpha_{3\mu}
\end{align*}
$$

(17)

for $s = x, y, z$. Derivatives of deformations $b$ and $f_s$ with respect to the laboratory variables $\alpha_{3\mu}$ are equal to

$$
\begin{align*}
    \frac{\partial b}{\partial \alpha_{3\mu}} &= (A_\mu(\omega))^* + \sum_{\nu, \omega} \frac{\partial}{\partial \omega} (A_{\nu}(\omega))^* \alpha_{3\nu} \frac{\partial \omega}{\partial \alpha_{3\mu}}, \\
    \frac{\partial f_s}{\partial \alpha_{3\mu}} &= (F_{\mu s}(\omega))^* + \sum_{\nu, \omega} \frac{\partial}{\partial \omega} (F_{\nu s}(\omega))^* \alpha_{3\nu} \frac{\partial \omega}{\partial \alpha_{3\mu}}
\end{align*}
$$

(18)

Derivatives of the Euler angles with respect to $\alpha_{3\mu}$ are obtained by solving the following set of linear equations:

$$
\sum_{\nu} \left[ \left( \frac{\partial}{\partial \varphi} (G_{\mu s}(\omega))^* \right) \frac{\partial \varphi}{\partial \alpha_{3\mu}} + \left( \frac{\partial}{\partial \theta} (G_{\nu s}(\omega))^* \right) \frac{\partial \theta}{\partial \alpha_{3\mu}} + \left( \frac{\partial}{\partial \psi} (G_{\nu s}(\omega))^* \right) \frac{\partial \psi}{\partial \alpha_{3\mu}} \right] \alpha_{3\nu} + (G_{\mu s}(\omega))^* = 0 \quad \text{for} \quad s = x, y, z.
$$

(19)

To calculate all the derivatives from Eqs. (18) and (19) one should calculate the derivatives of the octupole cubic Wigner functions with respect to the Euler angles. Using Eqs. (8) and (10) the derivatives of the cubic functions can be expressed by derivatives of the Wigner functions themselves. E.g., handbook contains formulae for the derivatives in question and other relevant properties of the Wigner
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Finally, solutions of Eq. (19) for derivatives of the Euler angles with respect to \( \alpha_{3\mu} \) are:

\[
\frac{\partial \varphi}{\partial \alpha_{3\mu}} = \frac{1}{2df(b, f_s)} \frac{1}{\sin \theta} \left[ -\cos \psi(\Gamma_{\mu x}(b, f_s, \omega))^* + \sin \psi(\Gamma_{\mu y}(b, f_s, \omega))^* \right]
\]

\[
\frac{\partial \theta}{\partial \alpha_{3\mu}} = \frac{1}{2df(b, f_s)} \left[ \sin \psi(\Gamma_{\mu x}(b, f_s, \omega))^* + \cos \psi(\Gamma_{\mu y}(b, f_s, \omega))^* \right]
\]

\[
\frac{\partial \psi}{\partial \alpha_{3\mu}} = \frac{1}{2df(b, f_s)} (\Gamma_{\mu z}(b, f_s, \omega))^* - \cos \theta \frac{\partial \varphi}{\partial \alpha_{3\mu}}
\]

(20)

where

\[
\Gamma_{\mu s}(b, f_x, f_y, f_z, \omega)^* = \frac{15}{16} f_x (G_{\mu x}(\omega))^* f_x - (G_{\mu t}(\omega))^* f_t - (G_{\mu u}(\omega))^* f_u
\]

\[
-\frac{\mu^2}{4} b (G_{\mu x}(\omega))^* + f_t (G_{\mu u}(\omega))^* \omega,
\]

(21)

and \( s, t, u \) are circular permutations of \( x, y, z \) here and further below. Using Eqs. (16), (18) and (20) we are in a position to express derivatives with respect to the laboratory by derivatives with respect to the intrinsic coordinates in the following two equivalent ways:

\[
\frac{\partial}{\partial \alpha_{3\mu}} = (A_\mu(\omega))^* \frac{\partial}{\partial b} + \sum_{s=x,y,z} \left\{ (F_{\mu s}(\omega))^* \frac{\partial}{\partial f_s} \right\}
\]

\[
+ \frac{i}{2df(b, f_x, f_y, f_z)} (\Gamma_{\mu s}(b, f_x, f_y, f_z, \omega))^* \left[ L_s(\omega) - J^{sf}(f_t, f_u) \right]
\]

\[
= \left[ \frac{\partial}{\partial b} + \frac{1}{df(b, f_x, f_y, f_z)} \frac{\partial df(b, f_x, f_y, f_z)}{\partial b} \right] (A_\mu(\omega))^*
\]

\[
+ \sum_{s=x,y,z} \left\{ \left[ \frac{\partial}{\partial f_s} + \frac{1}{df(b, f_x, f_y, f_z)} \frac{\partial df(b, f_x, f_y, f_z)}{\partial f_s} \right] (F_{\mu s}(\omega))^* \right\}
\]

(22)

where the differential operators

\[
J^{sf}(f_t, f_u) = \frac{3}{2} i \left( f_t \frac{\partial}{\partial f_u} - f_u \frac{\partial}{\partial f_t} \right)
\]

(23)

stand for angular momenta carried by vibrations of the octupole vector deformations \( f_x, f_y, f_z \) and will be called the octupole vibrational angular momenta.

Using both versions of the right-hand side of Eq. (22) and taking advantage of the unitarity of the octupole cubic Wigner functions we are able to express the Hamiltonian of Eq. (2) for \( \lambda = 3 \) in the intrinsic coordinates. To observe the inherent characteristics of the octupole collective motion an octupole Hamiltonian with the simplest inverse inertial bitensor, namely that of Eq. (5), will be presented here.

\[b\] Note that the Wigner functions from Ref. [28] are the complex conjugate of those used here.
This Hamiltonian when expressed in the Euler angles and octupole deformations is as follows:

\[
H_3(b, f_x, f_y, f_z, \omega) = -\frac{1}{2B_3} \sum_s \frac{\partial}{\partial f_s} H_3(b, f_x, f_y, f_z) \frac{\partial}{\partial f_s} - \sum_{s,s'} (L_s(\omega) - J_s^{(s)}(f_s, f_{s'})) \times d_s(b, f_x, f_y, f_z)(\tilde{I}^{(s)}(b, f_x, f_y, f_z))_{ss'}^{-1} \times (L_{s'}(\omega) - J_{s'}^{(s)}(f_{s'}, f_{s'})) + V(b, f_x, f_y, f_z)
\]

where the Cartesian tensor of the moments of inertia is equal to

\[
\tilde{I}^{(s)}(b, f_x, f_y, f_z) = \begin{pmatrix}
4b^2 + \frac{15}{4}(f_y^2 + f_z^2) & \frac{15}{4}f_x f_y + 2\sqrt{15}b f_z & \frac{15}{4}f_x f_z + 2\sqrt{15}b f_y \\
\frac{15}{4}f_x f_y + 2\sqrt{15}b f_z & 4b^2 + \frac{15}{4}(f_x^2 + f_z^2) & \frac{15}{4}f_y f_z + 2\sqrt{15}b f_x \\
\frac{15}{4}f_x f_z + 2\sqrt{15}b f_y & \frac{15}{4}f_y f_z + 2\sqrt{15}b f_x & 4b^2 + \frac{15}{4}(f_x^2 + f_y^2)
\end{pmatrix},
\]

It is seen that the intrinsic axes of an octupole system are not the principal axes of the moment of inertia as one would expect. The octupole vibrations, contrary to the quadrupole ones, carry their own angular momentum, which interacts by the Coriolis and centrifugal interactions with the total angular momentum (cf. Ref. [30]). This seems to be the most striking feature of the octupole rotations. In conclusion, the kinetic energy part of the Hamiltonian of Eq. (24) consists of ten terms: the four separate vibrations and the six rotational terms. In general, the Hamiltonian of Eq. (2) for \( \lambda = 3 \), when expressed in the intrinsic variables, can contain additionally six mixed vibrational terms of type \( \partial/\partial f_s \ldots \partial/\partial f_{s'} (s \neq s') \) and twelve vibration-rotation terms of type \( (\partial/\partial f_s \ldots (L_{s'} - J_{s'}^{(s)})) + \text{h.c.} \).

3.3. Axially-symmetric deformation

Many even-even nuclei show a static quadrupole deformation with axial symmetry. In the small-oscillations approximation of the collective Hamiltonian a simple picture of the quadrupole excitations has emerged (consult e.g. Chapter 6 in Ref. [29]). Two separate intrinsic vibrations appear, namely: the \( \beta \)-vibration of deformation \( a_{20} \approx \beta \) around the equilibrium deformation \( \beta_{eq} \), and the \( \gamma \)-vibration \( a_{22} \approx \beta \gamma \) strongly coupled to rotations around the symmetry axis. On the other hand, rotations around axes perpendicular to the symmetry axis are weakly coupled to the vibrations and form characteristic rotational bands built on top of every vibrational level.

How is it in the case of a static axially-symmetric octupole deformation? The equilibrium points in the four-dimensional deformation space are then supposed to be \( b = f_x = f_y = 0, f_z = \pm f_{eq} \). The equilibrium shape is shown in Fig. 2(a). A rough approximation of the small oscillations around the two (because of the mirror symmetry) equilibrium points for the Hamiltonian of Eq. (24) (with the
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original Bohr kinetic energy) reads as follows:

\[ H_3(b, f_x, f_y, f_z, \omega) \approx \sum_{s=x,y} \left[ -\frac{1}{2B_3} \frac{\partial^2}{\partial f_s^2} + \frac{1}{2} C_s f_s^2 \right] - \frac{1}{2B_3} \frac{\partial^2}{\partial f_z^2} + \frac{1}{2} C_z (|f_z| - |f_{eq}|)^2 + \frac{1}{2B_3} \left[ -\frac{1}{b} \frac{\partial}{\partial b} \frac{\partial}{\partial b} + \frac{(L_z(\omega) - J_s(f_x, f_y))^2}{4b^2} \right] + \frac{1}{2} C_b b^2 + \sum_{s=x,y} \frac{2}{15B_3 f_{eq}^2} (L_s(\omega) - J_s(f_x, f_y))^2 \]

From the form of the Hamiltonian given above the following pattern of the small oscillations around the axial-symmetric octupole shape emerges, namely:

- Two harmonic oscillations in coordinates \( f_x \) and \( f_y \) with stiffnesses \( C_x \) and \( C_y \), respectively (x- and y-vibrations),
- The double-oscillator z-vibrations around points \( f_z = \pm f_{eq} \) with stiffness \( C_z \) (cf. Ref. [31]),
- The \( b \)-vibration with stiffness \( C_b \) strongly coupled to rotation around the symmetry axis \( z \),
- Rotations around the x- and y-axes perpendicular to the symmetry axis with constant moment of inertia equal to \((15/4)B_3 f_{eq}^2\).

The rotations around the \( x \) and \( y \) axes form rotational bands on top of vibrational levels. However, the bands are disturbed by the Coriolis interaction, being a kind of the rotation-vibration interaction. In turn, centrifugal forces affect the four separate vibrations and can mix them with each other.

4. Conclusion

In the previous Sections a formalism for the octupole collective Hamiltonian has been presented and compared to that for the well-known quadrupole one. For a few reasons, like a number of degrees of freedom greater by two, negative parity, additional simplifications in the quadrupole case, the theory of the octupole collective Hamiltonian is essentially more complicated, and therefore less developed than that of the quadrupole collective motion. A substantial feature of the octupole motion, which does not seem to be realized, is that the intrinsic vector x-, y- and z-vibrations carry a non-zero angular momentum. This is obviously not the case for the quadrupole \( \beta \)- and \( \gamma \)-vibrations.

Obviously, a realistic collective model should take into account both modes, the quadrupole and the octupole together [19]. A separate consideration of the \( \lambda = 2 \) and \( \lambda = 3 \) cases either serves as a tool for developing a formalism and methods of treatment, or is an approximation. When we take, for instance, the kinetic energies of both modes with the Bohr inverse inertial bitensors of Eq. (5), the total
quadrupole-octupole Hamiltonian is the sum of the kinetic energies parametrized by the two mass parameters, $B_2$ and $B_3$, respectively, and the potential $V(\alpha_2, \alpha_3)$, which can contain a possible quadrupole-octupole interaction. However, modern collective Hamiltonians are extracted from microscopic theories, which seem to give inverse inertial bitensors $B^{-1}_{\lambda\mu\lambda'\mu'}(\alpha_2, \alpha_3)$ dependent on both sets of coordinates for both $\lambda$'s. Then, for instance, assumption no. (6) from Sec. 2 that the collective Hamiltonians contain isotropic functions of coordinates, is not valid. In consequence, the bitensor $B^{-1}_{2\mu3\nu}(\alpha_2, \alpha_3)$ can have more than six independent components. Furthermore, it is natural to allow for the appearance of mixed quadrupole-octupole terms in the total Hamiltonian. These terms would have the following form:

$$H_{23}(\alpha_2, \alpha_3) = -\frac{1}{2W(\alpha_2, \alpha_3)} \left[ \sum_{\mu,\nu} \frac{\partial}{\partial \alpha_{2\mu}} W(\alpha_2, \alpha_3)B^{-1}_{2\mu3\nu}(\alpha_2, \alpha_3) \frac{\partial}{\partial \alpha_{3\nu}} \right] + \sum_{\mu,\nu} \frac{\partial}{\partial \alpha_{3\mu}} W(\alpha_2, \alpha_3)B^{-1}_{3\mu2\nu}(\alpha_2, \alpha_3) \frac{\partial}{\partial \alpha_{2\nu}} + V_{23}(\alpha_2, \alpha_3).$$

(27)

Should $H_{23}$ be invariant under space inversion and Hermitian, $B^{-1}_{\lambda\mu\lambda'\mu'}(\alpha_2, \alpha_3)$ is symmetric ($\lambda\mu = \lambda'\mu'$) and odd. By analogy to Eq. (3) the mixed bitensor can be presented in the following form:

$$B^{-1}_{\lambda\mu\lambda'\mu'}(\alpha_2, \alpha_3) = 2 \sum_{l=0}^{2l+1m} (\lambda\mu\lambda'\mu' | 2l + 1m) T_{2l+1m}(\alpha_2, \alpha_3)$$

(28)

for $\lambda \neq \lambda' = 2, 3$. Tensors $T_{2l+1m}$ should have negative parity. The bitensor of Eq. (28) has 21 components altogether.

When the quadrupole-octupole collective Hamiltonian is considered assumptions nos. (1) – (6) from Sec. 2 should be extended to the collective space of both tensors, $\alpha_2$ and $\alpha_3$. The practical role of assumption no. (6) is that no material tensors appear for the nuclear medium. Under these extended assumptions the most general form of a quadrupole-octupole Hamiltonian reads as follows:

$$H(\alpha_2, \alpha_3) = -\frac{1}{2W(\alpha_2, \alpha_3)} \left[ \sum_{\lambda,\lambda'=2,3} \sum_{\mu,\mu'} \frac{\partial}{\partial \alpha_{\lambda\mu}} W(\alpha_2, \alpha_3)B^{-1}_{\lambda\mu\lambda'\mu'}(\alpha_2, \alpha_3) \frac{\partial}{\partial \alpha_{\lambda'\mu'}} \right] + V(\alpha_2, \alpha_3).$$

(29)

It is parametrized by 64 coordinate-dependent inertial functions being components of the three inverse inertial bitensors, scalar weight and potential. The weight can possibly be equal to the square root of the determinant of the $12 \times 12$ matrix of components of the inertial bitensors. The potential is a function of the coordinates through nine scalars described as deformations. In order to separate these nine variables from the twelve coordinates, a body-fixed intrinsic frame of reference and intrinsic coordinates have to be introduced. One can do this in different ways. For instance, the principal axes of tensor $\alpha_2$ oriented by the three Euler angles with
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respect to the laboratory axes can be treated as the intrinsic axes (cf. Ref. [19]). Then the two remaining intrinsic components of \( \alpha_2 \) and all the seven intrinsic components of \( \alpha_3 \) can be considered as deformations. Another way is to exchange the roles of tensors \( \alpha_2 \) and \( \alpha_3 \) and consider one of the frames defined in Sec. 3.1 through the octupole tensor as the intrinsic frame. One can also define two intrinsic frames for tensors \( \alpha_2 \) and \( \alpha_3 \) separately and treat the rotation of one frame with respect to the other as an intrinsic motion. Then the relative Euler angles have the status of deformations. Finally, in the case of a weak and well separated interaction between the modes one can treat them separately and then diagonalize the interaction within the product basis.

Only recently an attempt to solve a quadrupole-octupole model, similar to that presented here, however not based on Hamiltonian (29) and with a restricted number of degrees of freedom, has been undertaken [33]. The model has been applied to the positive- and negative-parity collective levels of the \(^{156}\)Gd nucleus. In any case, the problem of the full quadrupole-octupole collective Hamiltonian is apparently complicated enough and still awaits practical applications to the spectroscopy of nuclear collective excitations.

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Appendix A. Isotropic tensor fields in the octupole collective space

A.1. The positive spin-parity elementary tensors

The twelve positive spin-parity elementary tensors of Eq. (6) in the octupole collective space are as follows:

\[
\begin{align*}
  l = 0 & \quad t_0^{(2)}, t_0^{(4)}, t_0^{(6)}, t_0^{(10)}, \\
  l = 1 & \quad t_1^{(3)}, t_1^{(5)}, t_1^{(7)}, \\
  l = 2 & \quad t_2^{(2)}, t_2^{(4)}, \\
  l = 3 & \quad t_3^{(1)}, t_3^{(3)}, \\
  l = 4 & \quad t_4^{(2)}. 
\end{align*}
\]
A.2. Independent fundamental even tensors

Sets of fundamental even tensors with even ranks from 0 to 6 are listed in Table A.1. The choice of independent tensors need not be unique. This is because all fundamental tensors of a given rank (all possible alignments of the elementary tensors) are related to each other through a number of syzygies which can eliminate this or that tensor.

Table A.1. Fundamental even tensors with ranks $\Lambda = 0, 2, 4, 6$

| $\Lambda$ | $k_{3\Lambda}$ | $\tau_{k\Lambda}(\alpha_3)$ for $k = 1, \ldots, k_{3\Lambda}$ |
|-----------|----------------|-------------------------------------------------|
| 0         | 1              | $t_0^{(2)}$, $t_0^{(4)}$, $t_0^{(3)} \times t_0^{(3)}$, $t_0^{(3)} \times t_0^{(5)}$, $t_0^{(3)} \times t_0^{(7)}$ |
| 2         | 5              | $t_4^{(2)}$, $t_4^{(4)}$, $t_4^{(3)} \times t_4^{(3)}$, $t_4^{(3)} \times t_4^{(5)}$, $t_4^{(3)} \times t_4^{(7)}$ |
| 4         | 9              | $t_6^{(2)}$, $t_6^{(4)}$, $t_6^{(3)} \times t_6^{(3)}$, $t_6^{(3)} \times t_6^{(5)}$, $t_6^{(3)} \times t_6^{(7)}$ |
| 6         | 13             | $t_8^{(2)}$, $t_8^{(4)}$, $t_8^{(3)} \times t_8^{(3)}$, $t_8^{(3)} \times t_8^{(5)}$, $t_8^{(3)} \times t_8^{(7)}$ |

Appendix B. Symmetries of the coordinate frame

B.1. Cubic holohedral group

The cubic holohedral $O_h$ group 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. The three Bohr rotations, $R_1$, $R_2$, $R_3$, and the inversion $P$ can serve as generators of this group (see Ref. [15] and Sect. 4.4 in Ref. [29]). In general, the $O_h$ group has ten irreducible representations [32], namely

- four one-dimensional, denoted as $A_1^\pm$, $A_2^\pm$,
- two two-dimensional, denoted as $E^\pm$,
- four three-dimensional, denoted as $F_1^\pm$, $F_2^\pm$.

The tensor representations $D^\lambda$ of the $O(3)$ orthogonal group can be decomposed into the following irreducible representations of $O_h$, namely

- irreps $E^\pm$, $F_2^\pm$ for $\lambda = 2$,
- irreps $A_2^\pm$, $F_1^\pm$, $F_2^\pm$ for $\lambda = 3$.

B.2. Cubic coordinates

The decomposition of the real and imaginary parts, $a_{\lambda\mu}$, $b_{\lambda\mu}$ of the spherical components of tensors $\alpha_\lambda$ into cubic coordinates is:
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\( \lambda = 2 \)

\( E^+ \) \begin{cases} 
  e_{20} = a_{20} \\
  e_{22} = a_{22},
\end{cases} \quad \begin{cases} 
  f_{2x} = -b_{21}, \\
  g_{2y} = -a_{21}, \\
  g_{2z} = b_{22},
\end{cases} \tag{B.1}

\( \lambda = 3 \)

\[ A^+_2 : \ b_3 \equiv b = b_{32}, \]

\( F^+ \) \begin{cases} 
  f_{3x} \equiv f_x = \sqrt{\frac{3}{8}} a_{31} - \sqrt{\frac{5}{8}} a_{33}, \\
  f_{3y} \equiv f_y = \sqrt{\frac{3}{8}} b_{31} + \sqrt{\frac{5}{8}} b_{33}, \]

\[ f_{3z} \equiv f_z = a_{30}, \]

\( F^- \) \begin{cases} 
  g_{3x} \equiv g_x = \sqrt{\frac{3}{8}} a_{31} + \sqrt{\frac{5}{8}} a_{33}, \\
  g_{3y} \equiv g_y = -\sqrt{\frac{3}{8}} b_{31} + \sqrt{\frac{5}{8}} b_{33}, \]

\[ g_{3z} \equiv g_z = a_{32}, \tag{B.2} \]

Curly brackets match the cubic coordinates belonging to given irreducible representations of \( O_h \).

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