High Order Dependence of a Nuclear Rotation Hamiltonian

P. Yotov[1,2], N. Minkov[1,2], R. V. Jolos[3], and W. Scheid[2]

[1] Institute of Nuclear Research and Nuclear Energy, 72 Tzarigrad Road, Sofia 1784, Bulgaria
[2] Institut für Theoretische Physik der Justus-Liebig-Universität, Heinrich-Buff-Ring 16, D–35392 Giessen, Germany
[3] Joint Institute for Nuclear Research, 141980 Dubna, Russia

Abstract. A nuclear Hamiltonian with high order terms in the collective angular momentum operators is constructed by applying the method of contact transformations to a Hamiltonian including intrinsic particle motion and Coriolis interaction. In the space of intrinsic variables the coefficients of the transformed Hamiltonian appear as matrix elements depending on the intrinsic angular momentum. Their transformation properties under the time reversal assure the time-reversal invariance of the Hamiltonian in the collective space. The structure of the intrinsic matrix elements give an insight into the nature of these coefficients and justifies their appearance in various phenomenological collective Hamiltonians.

1 Introduction

The appearance of a high order angular momentum dependence in the rotation spectra of atomic nuclei is associated with the interaction between nuclear collective and intrinsic degrees of freedom [1]. The problem of the intrinsic origin of nuclear collective motion is a difficult one, and although extensive efforts to clarify it starting from "first principles" or from the more intuitive "geometric" aspect have been applied over the years, the obtained results suggest an unambiguous explanation of nuclear collective properties only in some particular cases [2–4].

In the simplest case of an axial symmetric nucleus with zero value $K = 0$ of the third projection of the collective angular momentum I, the leading order of the rotation Hamiltonian is $\hat{H}_{\text{rot}} = \hat{h}_0(\hat{I}_1^2 + \hat{I}_2^2)$, where $\hat{h}_0$ depends on intrinsic variables [1]. The expectation values of $\hat{H}_{\text{rot}}$ are given by the well known expression $E_{\text{rot}} = \hbar^2 I(I+1)/2\mathcal{J}$, with the moment of inertia given by $\mathcal{J} = (\hbar^2/2)\langle K = 0|\hat{h}_0|K=0\rangle^{-1}$.

In the general case of more complicated nuclear shape deformations including reflection asymmetry, triaxiality as well as deformations of larger multipolarity (octupole, hexadecapole, and so on) the high order angular momentum dependence of the total rotation Hamiltonian is not well studied. It has been shown that some basic properties of the rotating complex deformed system can be outlined by considering a generalized Hamiltonian of the form [5]

$$\hat{H}_I = h_0 + \sum_{\alpha} h_\alpha \hat{I}_\alpha + \sum_{\alpha,\beta} h_{\alpha\beta} \hat{I}_\alpha \hat{I}_\beta + \sum_{\alpha,\beta,\gamma} h_{\alpha\beta\gamma} \hat{I}_\alpha \hat{I}_\beta \hat{I}_\gamma + \cdots \ , \tag{1}$$

which is an infinite power series in the angular momentum components $\hat{I}_\alpha$ ($\alpha = x, y, z$) in the body fixed frame. The coefficients in (1) are supposed to depend on the intrinsic structure of the system. In principal they could be determined microscopically, for instance in the generalized density-matrix approach [6, 7]. However, this is a difficult task not yet solved in a way allowing a practical application. A simplification can be achieved if the vibration and rotation motion of the system are considered fully adiabatically separated. Then the Coriolis effects are absent from the rotational bands. In such a case the odd powers in the Hamiltonian (1) are excluded, $h_\alpha = h_{\alpha\beta\gamma} = \cdots = 0$, and thus only the centrifugal distortion effects are taken into account [5]. However, this is quite a simplified situation, especially, as regards to rotational spectra of complex deformed nuclei. From a geometric point of view the combinations of operators appearing in the various terms of (1) can be determined by using an appropriate point symmetry group (PSG) under certain assumptions for the shape characteristics of the system [5, 8]. In such a way some physically important properties of the system corresponding to complex shape deformations can be extracted from the expansion (1).

The purpose of the present work is to address the above problem by showing that a rotation Hamiltonian similar to (1) can be obtained in a diagonal form after applying the method of contact transformations [10, 11] to a Hamiltonian including intrinsic particle motion and Coriolis interaction. The coefficients of the transformed Hamiltonian are explicitly derived for the terms up to the third-power products of $\hat{I}^2$ and $\hat{I}_z$ in the form of operators depending on the intrinsic angular momentum. After acting in the space of intrinsic variables these coefficients appear as intrinsic matrix elements. Their symmetry properties under the time reversal ($\mathcal{T}$) operation provide the time-reversal invariance of the Hamiltonian in the collective space.

Various phenomenological collective models are developed by using Hamiltonians in the form of (1), where the coefficients are considered as fitting parameters [8, 9, 13]. Below it will be shown that the contact transformation approach reveals the physical meaning of these coefficients, as well as their dependence on the intrinsic structure of the system.

2 Derivation of a High Order Rotation Hamiltonian

Consider the Hamiltonian

$$\hat{H} = \hat{H}_p + \hat{H}_{\text{rot}} + \hat{H}_c, \tag{2}$$

where $\hat{H}_p$ describes the intrinsic motion of particles or quasiparticles in a mean field, $\hat{H}_{rot}$ is a pure rotation term

$$\hat{H}_{\text{rot}} = \frac{\hbar^2}{2\mathcal{J}} \hat{I}^2, \tag{3}$$

and $\hat{H}_c$ is the Coriolis interaction

$$\hat{H}_c = -\frac{\hbar^2}{2\mathcal{J}}(\hat{j}_+\hat{I}_- + \hat{j}_-\hat{I}_+), \tag{4}$$

where $\hat{I}_\pm = \hat{I}_x \pm \imath\hat{I}_y$, while $\hat{j}_\pm = \hat{j}_x \pm \imath\hat{j}_y$ are the spherical components of the total intrinsic particle angular momentum $\hat{j}$.

The part of the Hamiltonian (2) containing the intrinsic and the Coriolis interaction $\hat{h} \equiv (\hat{H}_p + \hat{H}_c)$ is not diagonal in the space of collective rotations $|I, I_z\rangle$. It can be, however, diagonalized by applying an unitary contact transformation [1, 10, 11] providing higher order angular momentum terms in the rotation part of the Hamiltonian. Below the prescription given in [12] is applied.

Consider the transformed operator

$$\hat{h}' \equiv \exp(\hat{T})\hat{h}\exp(-\hat{T}), \tag{5}$$

where the antihermitian operator $\hat{T}$ is defined in the form of an expansion $\hat{T} = \sum_n \hat{T}_n$ in which $n = 1, 2, 3, ...$ stands for the powers in which the raising and lowering components $\hat{I}_\pm$ of the total angular momentum appear in the respective members $\hat{T}_n$ of the expansion. The different operators $\hat{T}_n$ with $n = 1, 2, 3, ...$ are determined step by step (as it will be shown below), so as to keep only the diagonal terms of the transformed Hamiltonian $\hat{h}'$. To obtain the expansion up to some fixed degree n_f of the angular momentum components one has to expand the right hand side of Eq. (5) by using the formula

$$e^A B e^{-A} = B + [A, B] + \frac{1}{2}[A, [A, B]] + ... + \frac{1}{k!}\underbrace{[A, [A, ..., [}_{k \text{ brackets}} A, B]...]] + ...$$

and keeping only the terms up to the order n_f in $\hat{I}_\alpha$. Thus up to the fourth order ($n_f = 4$) one has

$$\begin{aligned}
\hat{h}' = {} & \hat{H}_p + \hat{H}_c + [\hat{T}_1,\, \hat{H}_p] + \\
& + [\hat{T}_2,\, \hat{H}_p] + [\hat{T}_1,\, \hat{H}_c] + \frac{1}{2}[\hat{T}_1, [\hat{T}_1,\, \hat{H}_p]] + \\
& + [\hat{T}_3,\, \hat{H}_p] + [\hat{T}_2,\, \hat{H}_c] + \frac{1}{2}[\hat{T}_2, [\hat{T}_1,\, \hat{H}_p]] + \\
& + \frac{1}{2}[\hat{T}_1, [\hat{T}_2,\, \hat{H}_p]] + \frac{1}{2}[\hat{T}_1, [\hat{T}_1,\, \hat{H}_c]] + \frac{1}{6}[\hat{T}_1, [\hat{T}_1, [\hat{T}_1,\, \hat{H}_p]]] + \\
& + [\hat{T}_4,\, \hat{H}_p] + [\hat{T}_3,\, \hat{H}_c] + \frac{1}{2}[\hat{T}_1, [\hat{T}_3,\, \hat{H}_p]] + \\
& + \frac{1}{2}[\hat{T}_2, [\hat{T}_2,\, \hat{H}_p]] + \frac{1}{2}[\hat{T}_3, [\hat{T}_1,\, \hat{H}_p]] + \\
& + \frac{1}{2}[\hat{T}_1, [\hat{T}_2,\, \hat{H}_c]] + \frac{1}{2}[\hat{T}_2, [\hat{T}_1,\, \hat{H}_c]] + \frac{1}{6}[\hat{T}_1, [\hat{T}_1, [\hat{T}_1,\, \hat{H}_c]]] + \\
& + \frac{1}{6}[\hat{T}_1, [\hat{T}_1, [\hat{T}_2,\, \hat{H}_p]]] + \frac{1}{6}[\hat{T}_1, [\hat{T}_2, [\hat{T}_1,\, \hat{H}_p]]] + \\
& + \frac{1}{6}[\hat{T}_2, [\hat{T}_1, [\hat{T}_1,\, \hat{H}_p]]] + \frac{1}{24}[\hat{T}_1, [\hat{T}_1, [\hat{T}_1, [\hat{T}_1,\, \hat{H}_p]]]].
\end{aligned} \tag{6}$$

As a first step, the operator $\hat{T}_1$ is determined by the relation

$$[\hat{T}_1,\, \hat{H}_p] = -\hat{H}_c = \frac{\hbar^2}{2\mathcal{J}}(\hat{j}_+\hat{I}_- + \hat{j}_-\hat{I}_+), \tag{7}$$

which eliminates the first order contribution of the nondiagonal Coriolis term $\hat{H}_c$ in Eq. (6). This relation suggests that $\hat{T}_1$ can be taken in the form

$$\hat{T}_1 = (\hat{\varepsilon}_+\hat{I}_- - \hat{\varepsilon}_-\hat{I}_+), \tag{8}$$

where the operators $\hat{\varepsilon}_\pm$ are functions of the intrinsic degrees of freedom and satisfy the commutation relations

$$[\hat{\varepsilon}_\pm,\, \hat{H}_p] = \pm\frac{\hbar^2}{2\mathcal{J}}\hat{j}_\pm. \tag{9}$$

(We remark that the expression (8) is used in [1].)

In the second step, the operator $\hat{T}_2$ is determined so as to eliminate the nondiagonal contribution of the second order operator $[\hat{T}_1, \hat{H}_c]$, namely

$$[\hat{T}_2,\, \hat{H}_p] = -\frac{1}{2}[\hat{T}_1,\, \hat{H}_c]_{\text{nd}}, \tag{10}$$

where 'nd' means 'nondiagonal part'. The operator $[\hat{T}_1, \hat{H}_c]_{\text{nd}}$ can be obtained explicitly as a linear combination of the second order operators $\hat{I}_\pm^2$. It allows one to suppose, by analogy to $\hat{T}_1$, the form of the operator $\hat{T}_2$ as a function of $\hat{I}_\pm^2$

$$\hat{T}_2 = \hat{\delta}_+\hat{I}_-^2 + \hat{\delta}_-\hat{I}_+^2. \tag{11}$$

As a consequence of Eq. (10), the operators $\hat{\delta}_\pm$ are determined by the commutation relations

$$[\hat{\delta}_\pm,\, \hat{H}_p] = \frac{\hbar^2}{2\mathcal{J}}[\hat{\varepsilon}_\pm,\, \hat{j}_\pm]. \tag{12}$$

Similarly to the previous two steps the operator $\hat{T}_3$ is determined by

$$[\hat{T}_3,\, \hat{H}_p] = -\left(\frac{1}{2}[\hat{T}_2,\, \hat{H}_c] - \frac{1}{4}[\hat{T}_1, [\hat{T}_1\, \hat{H}_c]_{\text{nd}}] + \frac{1}{3}[\hat{T}_1, [\hat{T}_1\, \hat{H}_c]]\right)_{\text{nd}}, \tag{13}$$

so as to eliminate the third order non-diagonal terms. As a result it can be presented in the form

$$\begin{aligned}\hat{T}_3 = {} & \hat{\sigma}_+^{(0)}\hat{I}_- - \hat{\sigma}_-^{(0)}\hat{I}_+ + \\ & + \hat{\sigma}_+^{(1)}\{\hat{I}_z,\, \hat{I}_-\} - \hat{\sigma}_-^{(1)}\{\hat{I}_z,\, \hat{I}_+\} + \\ & + \hat{\gamma}_+^{(0)}\hat{I}_-^3 - \hat{\gamma}_-^{(0)}\hat{I}_+^3 + \\ & + \hat{\gamma}_+^{(1)}\{\hat{I}^2 - \hat{I}_z^2,\, \hat{I}_-\} - \hat{\gamma}_-^{(1)}\{\hat{I}^2 - \hat{I}_z^2,\, \hat{I}_+\},\end{aligned} \tag{14}$$

where the intrinsic operators $\hat{\sigma}_{\pm}^{(0),(1)}$ and $\hat{\gamma}_{+}^{(0),(1)}$ are determined by the commutation relations

$$[\hat{\sigma}_{\pm}^{(0)},\,\hat{H}_p] = -\frac{\hbar^2}{2\mathcal{J}}\left(\pm\frac{1}{4}[\hat{\delta}_{\pm},\hat{j}_{\mp}] \mp \frac{1}{24}[\hat{\varepsilon}_{\mp},\hat{\tau}_{\pm}^{(0)}] \pm \frac{1}{6}\{\hat{\varepsilon}_{\pm},\hat{\tau}_1\}\right) \tag{15}$$

$$[\hat{\sigma}_{\pm}^{(1)},\,\hat{H}_p] = -\frac{\hbar^2}{2\mathcal{J}}\left(-\frac{1}{2}\{\hat{\delta}_{\pm},j_{\mp}\} - \frac{1}{12}\{\hat{\varepsilon}_{\mp},\hat{\tau}_{\pm}^{(0)}\} \mp \frac{1}{6}\hat{\tau}_{\pm}\right) \tag{16}$$

$$[\hat{\gamma}_{\pm}^{(0)},\,\hat{H}_p] = -\frac{\hbar^2}{2\mathcal{J}}\left(-[\hat{\delta}_{\pm},\hat{j}_{\pm}] - \frac{1}{12}[\hat{\varepsilon}_{\pm},\hat{\tau}_{\pm}^{(0)}]\right) \tag{17}$$

$$[\hat{\gamma}_{\pm}^{(1)},\,\hat{H}_p] = -\frac{\hbar^2}{2\mathcal{J}}\left(\mp\frac{1}{4}[\hat{\delta}_{\pm},\hat{j}_{\mp}] \pm \frac{1}{24}[\hat{\varepsilon}_{\mp},\hat{\tau}_{\pm}^{(0)}] - \frac{1}{6}[\hat{\varepsilon}_{\pm},\hat{\tau}_2]\right), \tag{18}$$

with

$$\hat{\tau}_1 = \{\hat{\varepsilon}_+,\hat{j}_-\} + \{\hat{\varepsilon}_-,\hat{j}_+\} \qquad \hat{\tau}_2 = [\hat{\varepsilon}_+,\hat{j}_-] - [\hat{\varepsilon}_-,\hat{j}_+] \tag{19}$$

and

$$\hat{\tau}_{\pm}^{(0)} = [\hat{\varepsilon}_{\pm},\hat{j}_{\pm}] \qquad \hat{\tau}_{\pm}^{(1)} = \pm[\hat{\varepsilon}_{\pm},\hat{\tau}_1] + \{\hat{\varepsilon}_{\pm},\hat{\tau}_2\}. \tag{20}$$

In the above the curly brackets mean anticommutation ($\{A,B\} \equiv AB + BA$).

Finally, the operator $\hat{T}_4$ is determined through the commutation relation

$$\begin{aligned}
[\hat{T}_4,\,\hat{H}_p] = &-\frac{1}{2}[\hat{T}_3,\,\hat{H}_c]_{\text{nd}} - \frac{1}{3}[\hat{T}_1,[\hat{T}_2,\,\hat{H}_c]]_{\text{nd}} - \frac{1}{3}[\hat{T}_2,[\hat{T}_1,\,\hat{H}_c]]_{\text{nd}} \\
&+ \frac{1}{4}[\hat{T}_1,[\hat{T}_2,\,\hat{H}_c]_{\text{nd}}]_{\text{nd}} + \frac{1}{4}[\hat{T}_2,[\hat{T}_1,\,\hat{H}_c]_{\text{nd}}]_{\text{nd}} \\
&- \frac{1}{8}[\hat{T}_1,[\hat{T}_1,[\hat{T}_1,\,\hat{H}_c]_{\text{nd}}]_{\text{nd}}]_{\text{nd}} + \frac{1}{6}[\hat{T}_1,[\hat{T}_1,[\hat{T}_1,\,\hat{H}_c]]_{\text{nd}}]_{\text{nd}} \\
&+ \frac{1}{12}[\hat{T}_1,[\hat{T}_1,[\hat{T}_1,\,\hat{H}_c]_{\text{nd}}]]_{\text{nd}} - \frac{1}{8}[\hat{T}_1,[\hat{T}_1,[\hat{T}_1,\,\hat{H}_c]]]_{\text{nd}}\,,
\end{aligned} \tag{21}$$

so as to eliminate all remaining (fourth order) nondiagonal terms in Eq. (6). As a result, the transformed Hamiltonian appears in the form

$$\begin{aligned}
\hat{h}' = \hat{H}_p &+ \frac{1}{2}[\hat{T}_1,\,\hat{H}_c]_{\text{d}} + \frac{1}{2}[\hat{T}_2,\,\hat{H}_c]_{\text{d}} + \frac{1}{2}[\hat{T}_3,\,\hat{H}_c]_{\text{d}} \\
&+ \frac{1}{3}[\hat{T}_1,[\hat{T}_1,\,\hat{H}_c]]_{\text{d}} + \frac{1}{3}[\hat{T}_1,[\hat{T}_2,\,\hat{H}_c]]_{\text{d}} + \frac{1}{3}[\hat{T}_2,[\hat{T}_1,\,\hat{H}_c]]_{\text{d}} \\
&- \frac{1}{4}[\hat{T}_1,[\hat{T}_1,\,\hat{H}_c]_{\text{nd}}]_{\text{d}} - \frac{1}{4}[\hat{T}_1,[\hat{T}_2,\,\hat{H}_c]_{\text{nd}}]_{\text{d}} - \frac{1}{4}[\hat{T}_2,[\hat{T}_1,\,\hat{H}_c]_{\text{nd}}]_{\text{d}} \\
&+ \frac{1}{8}[\hat{T}_1,[\hat{T}_1,[\hat{T}_1,\,\hat{H}_c]_{\text{nd}}]_{\text{nd}}]_{\text{d}} - \frac{1}{6}[\hat{T}_1,[\hat{T}_1,[\hat{T}_1,\,\hat{H}_c]]_{\text{nd}}]_{\text{d}} \\
&- \frac{1}{12}[\hat{T}_1,[\hat{T}_1,[\hat{T}_1,\,\hat{H}_c]_{\text{nd}}]]_{\text{d}} + \frac{1}{8}[\hat{T}_1,[\hat{T}_1,[\hat{T}_1,\,\hat{H}_c]]]_{\text{d}}\,,
\end{aligned} \tag{22}$$

where ‘d’ means ‘diagonal part’.

Then, after using the explicit dependence of the operators $\hat{T}_1$, $\hat{T}_2$ and $\hat{T}_3$ on the powers of the operators $\hat{I}_{\pm}$ and $\hat{I}_z$ [Eqs (8), (11) and (14), respectively] with all related commutation relations, the transformed Hamiltonian $\hat{h}'$ can be written up to the third order as

$$\hat{h}' \equiv \exp(\hat{T})\hat{h}\exp(-\hat{T}) = \hat{H}_p + \hat{t}_1\hat{I}_z + \hat{t}_2\hat{I}_z^2 + \hat{t}'_2(\hat{I}^2 - \hat{I}_z^2) + \hat{t}'_3(\hat{I}^2 - \hat{I}_z^2)\hat{I}_z + \ldots \quad (23)$$

The coefficients in the expansion (23) depend on the total intrinsic angular-momentum operators $\hat{j}_\pm$ and on operators defined recursively through commutation relations with $\hat{H}_p$. The operator-coefficients $\hat{t}_1$, $\hat{t}_2$, $\hat{t}'_2$ and $\hat{t}'_3$ have been derived in the following explicit form

$$\begin{aligned}
\hat{t}_1 = -\frac{\hbar^2}{2\mathcal{J}} \Bigg(& \frac{1}{2}(\{\hat{\varepsilon}_+, \hat{j}_-\} + \{\hat{\varepsilon}_-, \hat{j}_+\}) - (\{\hat{\sigma}_+^{(0)}, \hat{j}_-\} + \{\hat{\sigma}_-^{(0)}, \hat{j}_+\}) \\
& + (\{\hat{\gamma}_+^{(1)}, \hat{j}_-\} + \{\hat{\gamma}_-^{(1)}, \hat{j}_+\}) + ([\hat{\sigma}_+^{(1)}, \hat{j}_-] - [\hat{\sigma}_-^{(1)}, \hat{j}_+]) \\
& + \frac{1}{6}(\{\hat{\delta}_+, \hat{\tau}_-^{(0)}\} - \{\hat{\delta}_-, \hat{\tau}_+^{(0)}\}) + ([\hat{\varepsilon}_+, \hat{\delta}_-^{(2)}] + [\hat{\varepsilon}_-, \hat{\delta}_+^{(2)}]) \\
& + \frac{1}{48}([\hat{\varepsilon}_+, \hat{\tau}_-^{(1)}] - [\hat{\varepsilon}_-, \hat{\tau}_+^{(1)}]) + \frac{1}{48}(\{\hat{\varepsilon}_+, \hat{\varepsilon}_-^{(12)}\} + \{\hat{\varepsilon}_-, \hat{\varepsilon}_+^{(12)}\}) \\
& - \frac{1}{48}(\{\hat{\varepsilon}_+, \hat{\varepsilon}_-^{(21)}\} - \{\hat{\varepsilon}_-, \hat{\varepsilon}_+^{(21)}\}) \Bigg)
\end{aligned} \quad (24)$$

$$\begin{aligned}
\hat{t}_2 = -\frac{\hbar^2}{2\mathcal{J}} \Bigg(& 2(\{\hat{\sigma}_+^{(1)}, \hat{j}_-\} + \{\hat{\sigma}_-^{(1)}, \hat{j}_+\}) - \frac{1}{4}([\hat{\delta}_+, \hat{\tau}_-^{(0)}] - [\hat{\delta}_-, \hat{\tau}_+^{(0)}]) \\
& - \frac{1}{12}([\hat{\varepsilon}_+, \hat{\delta}_-^{(1)}] - [\hat{\varepsilon}_-, \hat{\delta}_+^{(1)}]) + \frac{1}{6}(\{\hat{\varepsilon}_+, \hat{\delta}_-^{(2)}\} - \{\hat{\varepsilon}_-, \hat{\delta}_+^{(2)}\}) \\
& + \frac{1}{24}([\hat{\varepsilon}_+, \hat{\varepsilon}_-^{(21)}] + [\hat{\varepsilon}_-, \hat{\varepsilon}_+^{(21)}]) + \frac{1}{24}(\{\hat{\varepsilon}_+, \hat{\tau}_-^{(1)}\} + \{\hat{\varepsilon}_-, \hat{\tau}_+^{(1)}\}) \\
& + 2([\hat{\gamma}_+^{(1)}, \hat{j}_-] - [\hat{\gamma}_-^{(1)}, \hat{j}_+]) \Bigg)
\end{aligned} \quad (25)$$

$$\begin{aligned}
\hat{t}'_2 = -\frac{\hbar^2}{2\mathcal{J}} \Bigg(& ([\hat{\varepsilon}_+, \hat{j}_-] - [\hat{\varepsilon}_-, \hat{j}_+]) + \frac{1}{12}([\hat{\delta}_+, \hat{\tau}_-^{(0)}] - [\hat{\delta}_-, \hat{\tau}_+^{(0)}]) \\
& - \frac{1}{12}(\{\hat{\varepsilon}_+, \hat{\delta}_-^{(2)}\} - \{\hat{\varepsilon}_-, \hat{\delta}_+^{(2)}\}) + \frac{1}{48}([\hat{\varepsilon}_+, \hat{\varepsilon}_-^{(12)}] - [\hat{\varepsilon}_-, \hat{\varepsilon}_+^{(12)}]) \\
& + \frac{1}{48}([\hat{\varepsilon}_+, \hat{\varepsilon}_-^{(21)}] + [\hat{\varepsilon}_-, \hat{\varepsilon}_+^{(21)}]) - \frac{1}{48}(\{\hat{\varepsilon}_+, \hat{\tau}_-^{(1)}\} + \{\hat{\varepsilon}_-, \hat{\tau}_+^{(1)}\}) \\
& - ([\hat{\sigma}_+^{(0)}, \hat{j}_-] - [\hat{\sigma}_-^{(0)}, \hat{j}_+]) - ([\hat{\gamma}_+^{(1)}, \hat{j}_-] - [\hat{\gamma}_-^{(1)}, \hat{j}_+])) \\
& - (\{\hat{\sigma}_+^{(1)}, \hat{j}_-\} + \{\hat{\sigma}_-^{(1)}, \hat{j}_+\}) \Bigg)
\end{aligned} \quad (26)$$

$$\begin{aligned}\hat{t}'_3 = -\frac{\hbar^2}{2\mathcal{J}}\Big(&-2([\hat{\sigma}_+^{(1)},\hat{j}_-]-[\hat{\sigma}_-^{(1)},\hat{j}_+]) - 2(\{\hat{\gamma}_+^{(1)},\hat{j}_-\}+\{\hat{\gamma}_-^{(1)},\hat{j}_+\})\\ &-\frac{1}{2}(\{\hat{\delta}_+,\hat{\tau}_-^{(0)}\}+\{\hat{\delta}_-,\hat{\tau}_+^{(0)}]) - \frac{1}{6}([\hat{\varepsilon}_+,\hat{\delta}_-^{(2)}]+[\hat{\varepsilon}_-,\hat{\delta}_+^{(2)}])\\ &+\frac{1}{12}(\{\hat{\varepsilon}_+,\hat{\delta}_-^{(1)}\}+\{\hat{\varepsilon}_-,\hat{\delta}_+^{(1)}\}) - \frac{1}{24}([\hat{\varepsilon}_+,\hat{\tau}_-^{(0)}]-[\hat{\varepsilon}_-,\hat{\tau}_+^{(0)}])\\ &+\frac{1}{12}(\{\hat{\varepsilon}_+,\hat{\varepsilon}_-^{(21)}\}-\{\hat{\varepsilon}_-,\hat{\varepsilon}_+^{(12)}\})\Big)\end{aligned} \tag{27}$$

with

$$\hat{\delta}_\pm^{(0)} = [\hat{\delta}_\pm,\hat{j}_\pm], \qquad \hat{\delta}_\pm^{(1)} = [\hat{\delta}_\pm,\hat{j}_\mp], \qquad \hat{\delta}_\pm^{(2)} = \{\hat{\delta}_\pm,\hat{j}_\mp\} \tag{28}$$

$$\hat{\varepsilon}_\pm^{(12)} = \{\hat{\varepsilon}_\pm,\hat{\tau}_1\}, \qquad \hat{\varepsilon}_\pm^{(21)} = [\hat{\varepsilon}_\pm,\hat{\tau}_2]. \tag{29}$$

3 Properties of the Hamiltonian in the Collective Space

The above derived high order expansion (23) allows one to discuss the properties of a more general non-diagonal Hamiltonian, given in the form

$$\hat{H}_{t,I} = \hat{t}_0 + \sum_\alpha \hat{t}_\alpha \hat{I}_\alpha + \sum_{\alpha,\beta} \hat{t}_{\alpha\beta}\hat{I}_\alpha\hat{I}_\beta + \sum_{\alpha,\beta,\gamma} \hat{t}_{\alpha\beta\gamma}\hat{I}_\alpha\hat{I}_\beta\hat{I}_\gamma + \sum_{\alpha,\beta,\gamma,\delta} \hat{t}_{\alpha\beta\gamma\delta}\hat{I}_\alpha\hat{I}_\beta\hat{I}_\gamma\hat{I}_\delta + \cdots . \tag{30}$$

This Hamiltonian is an analogue of (1), but similarly to (23) the coefficients $\hat{t}_\xi$ ($\xi = \alpha, \alpha\beta, \alpha\beta\gamma, ...$) in the different angular momentum powers $\prod_\kappa \hat{I}_\kappa$ ($\kappa = \alpha, \beta, \gamma, ...$) represent operators acting in the space of intrinsic variables. The Hamiltonian (1) can be obtained through the action of (30) in the intrinsic space as follows. Consider that the total wave function of the nucleus can be taken in the form

$$\Psi \sim |\tau\Omega\rangle|IKM\rangle, \tag{31}$$

where $|IKM\rangle$ is the standard collective part (M is the third projection of $\hat{I}$ in the laboratory frame) and $|\tau\Omega\rangle$ is the intrinsic part characterized by the third projection Ω of the intrinsic angular momentum $\hat{j}$ in the body fixed frame (τ stands for other intrinsic quantum numbers). In the strong coupling limit Ω and K are related and moreover in the well deformed axially symmetric nuclei one has $K = \Omega$ [2]. Here, however, no explicit relation between K and Ω is imposed, keeping the validity of the consideration for the cases of non-axial deformations and of a weak coupling between the intrinsic and collective degrees of freedom. Hence one can assume that the intrinsic operator-coefficients $\hat{t}_\xi$ in (30) act only in the intrinsic space $|\tau\Omega\rangle$, while the angular momentum powers $\prod_\kappa \hat{I}_\kappa$ act only in the collective space

$|IKM\rangle$. Then by taking the expectation value of the total Hamiltonian $\hat{H}_{t,I}$ in a given intrinsic state $|\tau\Omega_0\rangle$ one obtains a collective Hamiltonian of the form (1)

$$\hat{H}_{\text{coll}} = \langle\tau\Omega_0|\hat{H}_{t,I}|\tau\Omega_0\rangle = h_0 + \sum_{\alpha} h_\alpha \hat{I}_\alpha + \sum_{\alpha,\beta} h_{\alpha\beta}\hat{I}_\alpha\hat{I}_\beta$$
$$+ \sum_{\alpha,\beta,\gamma} h_{\alpha\beta\gamma}\hat{I}_\alpha\hat{I}_\beta\hat{I}_\gamma + \sum_{\alpha,\beta,\gamma,\delta} h_{\alpha\beta\gamma\delta}\hat{I}_\alpha\hat{I}_\beta\hat{I}_\gamma\hat{I}_\delta + \cdots \,, \qquad (32)$$

where

$$\begin{aligned} h_0 &\equiv \langle\tau\Omega_0|\hat{t}_0|\tau\Omega_0\rangle, \qquad h_\alpha \equiv \langle\tau\Omega_0|\hat{t}_\alpha|\tau\Omega_0\rangle, \\ h_{\alpha\beta} &\equiv \langle\tau\Omega_0|\hat{t}_{\alpha\beta}|\tau\Omega_0\rangle, \;\; h_{\alpha\beta\gamma} \equiv \langle\tau\Omega_0|\hat{t}_{\alpha\beta\gamma}|\tau\Omega_0\rangle, \\ h_{\alpha\beta\gamma\delta} &\equiv \langle\tau\Omega_0|\hat{t}_{\alpha\beta\gamma\delta}|\tau\Omega_0\rangle \end{aligned} \qquad (33)$$

represent intrinsic matrix elements. In principal the matrix elements (33) can be calculated, if the explicit form of the operators $\hat{t}_\xi$ $(\xi = \alpha, \alpha\beta, \alpha\beta\gamma, ...)$ is given, as in the particular case of Eqs. (24)–(27). A simple example up to the second order is given in [12]. By considering $\Omega_0 = K$ and having in mind Eq. (22) of [12] one has

$$\langle K|\hat{t}_1|K\rangle \sim \frac{\langle K|j_+|K-1\rangle^2}{E_K - E_{K-1}} + \frac{\langle K+1|j_+|K\rangle^2}{E_{K+1} - E_K} \qquad (34)$$

$$\langle K|\hat{t}_2|K\rangle \sim \frac{\langle K|j_+|K-1\rangle^2}{E_K - E_{K-1}} - \frac{\langle K+1|j_+|K\rangle^2}{E_{K+1} - E_K}, \qquad (35)$$

where E_K is the intrinsic particle energy.

Here, the following comments on the odd angular momentum powers appearing in the transformed Hamiltonian (23) as well as in the more general collective Hamiltonian (32) should take place. It is obvious that terms as $\hat{I}_z$, $\hat{I}_z^3$ and $\hat{I}^2\hat{I}_z$ entering (23), are not invariant under the time reversal transformation. On the other hand, since the initial Hamiltonian (2) is a time reversal invariant and the contact transformation does not affect the time reversal symmetry, one should expect that the transformed Hamiltonian is also an invariant. Indeed, by using the explicit expressions (24) and (27), it can be verified that the respective intrinsic operator-coefficients $\hat{t}_1$ and $\hat{t}'_3$ in (23) are not invariant under the time reversal. Thus it appears that the corresponding terms in the expansion (23)represent products of two (intrinsic and collective) non-invariant (time-odd) operators under the time reversal. Since the product of two time-odd operators is a time-even operator, it is proved that the transformed Hamiltonian is a time reversal invariant. In the case of even angular momentum powers one has products of two time-even operators which also assure the time reversal invariance of the Hamiltonian.

In a similar way the time reversal invariance of the Hamiltonian (32) is provided by the transformation properties of the coefficients h_ξ which represent intrinsic matrix elements. One deduces that the matrix elements corresponding to the odd angular momentum powers change in sign under the time reversal and together with the simultaneous change in the sign of the collective time-odd operators assure the invariance of the collective Hamiltonian. Thus, for the odd powers in (32) one has the sign inversion property

$$h_\alpha \xrightarrow{\mathcal{T}} -h_\alpha \qquad h_{\alpha\beta\gamma} \xrightarrow{\mathcal{T}} -h_{\alpha\beta\gamma}. \tag{36}$$

The matrix elements in the even angular momentum powers do not change in sign.

Since the operators $\hat{t}_\xi$ are hermitian, the coefficients h_ξ obtain real values. Therefore, the collective Hamiltonian of the form (32) is both, hermitian and time reversal invariant. One should, however, keep in mind that the coefficients h_ξ are not simply numbers, but matrix elements of intrinsic operators. Therefore, their values, although being real numbers, can appear with changed signs, as in (36), after the time reversal operation is applied. This can be easily illustrated for the terms $\hat{t}_1\hat{I}_z$ and $\hat{t}_2\hat{I}_z^2$ in Eq. (23) by using Eqs. (34) and (35). Since the intrinsic particle Hamiltonian is a time reversal invariant, one has for the single particle energy $E_K = E_{-K}$. Then, it is clear that under time reversal operation, with $K \xrightarrow{\mathcal{T}} -K$, the matrix element $\langle K|\hat{t}_1|K\rangle$, Eq. (34), changes in sign (time-odd), while the matrix element $\langle K|\hat{t}_2|K\rangle$, Eq. (35) does not change (time-even). These properties together with the symmetries of the operators $\hat{I}_z$ (time-odd) and $\hat{I}_z^2$ (time-even) provide the time reversal invariance of the considered Hamiltonian terms. Since after being calculated the intrinsic matrix elements Eqs. (34) and (35) give real numbers and the operator $\hat{I}_z$ is hermitian, the respective collective Hamitonian terms are also hermitian.

4 Concluding Remarks

The contact transformation formalism developed in the present work allows the derivation of high order angular momentum terms in the nuclear rotation Hamiltonian by taking into account the interplay between collective and intrinsic degrees of freedom. It is shown that the intrinsic (microscopic) origin of the coefficients in the different angular momentum powers provides the correct transformation properties of the Hamiltonian under time reversal and imposes specific sign inversion rules when the consideration is restricted to the collective space. On this basis the following main goals are achieved in the present work:

i) The method of contact transformations can be of essential use in the subject of collective nuclear structure.

ii) It is shown that Hamiltonian terms containing odd powers of the collective angular momentum operators can play an important role in nuclear dynamics after taking appropriately into account the presence of intrinsic degrees of freedom.

iii) It is suggested that collective models based on expansions in the powers of the angular momentum can be justified on a deeper microscopic level by connecting the expansion coefficients to the matrix elements of operators acting in the space of intrinsic nuclear variables.

Based on the Coriolis-type interaction between intrinsic and collective modes the presented formalism allows us to gain an insight into the origin of some basic properties of nuclear dynamics. From the intrinsic point of view the various degrees of freedom are incorporated in the intrinsic matrix elements, which carry information about the ability of the microscopic structure to “support” a given rotation mode. From the collective point of view different high order products of angular momentum components give respective input in the rotation properties of the system. From the fundamental-invariance point of view the collective and intrinsic parts of the Hamiltonian terms are strictly determined so as to ensure the time reversal invariance of the total Hamiltonian.

In conclusion, the construction of the nuclear rotation Hamiltonian including high order angular momentum terms with microscopically determined coefficients suggests a theoretical tool in the study of the intrinsic origin of nuclear collective motion.

Acknowledgments

We thank S. B. Drenska for valuable discussions. This work is supported by DFG and by the Bulgarian Scientific Fund under contract F-1502/05.

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