# Higher-rank discrete symmetries in the IBM. I Octahedral shapes: general Hamiltonian 

P. van Isacker, A. Bouldjedri, S. Zerguine

## - To cite this version:

P. van Isacker, A. Bouldjedri, S. Zerguine. Higher-rank discrete symmetries in the IBM. I Octahedral shapes: general Hamiltonian. Nuclear Physics A, 2015, 938, pp.45-58. 10.1016/j.nuclphysa.2015.03.003 . in2p3-01127998

HAL Id: in2p3-01127998
https://hal.in2p3.fr/in2p3-01127998
Submitted on 9 Mar 2015

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire HAL, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

# Higher-rank discrete symmetries in the IBM. I Octahedral shapes: general Hamiltonian 

P. Van Isacker, ${ }^{\text {a }}$ A. Bouldjedri ${ }^{\text {b }}$ and S. Zerguine ${ }^{\text {b }}$<br>${ }^{\text {a }}$ Grand Accélérateur National d'Ions Lourds, CEA/DSM-CNRS/IN2P3<br>Bd Henri Becquerel, BP 55027, F-14076 Caen Cedex 5, France<br>${ }^{\mathrm{b}}$ Department of Physics, PRIMALAB Laboratory, University of Batna Avenue Boukhelouf M El Hadi, 05000 Batna, Algeria


#### Abstract

In the context of the interacting boson model with $s, d$ and $g$ bosons, the conditions for obtaining an intrinsic shape with octahedral symmetry are derived for a general Hamiltonian with up to two-body interactions.


Key words: discrete octahedral symmetry, interacting boson model, $g$ bosons PACS: 21.60.Ev, 21.60.Fw

## 1 Introduction

The collective model of the atomic nucleus assumes a description in terms of the shape of a surface and its oscillations around that shape. In nuclei quadrupole deformations with multipolarity $\lambda=2$ parameterize the most important deviation from spherical shape. Their manifestation, either as a vibration around a spherical shape or through the mechanism of spontaneous symmetry breaking as a permanent deformation, is by now a widely accepted feature of nuclear structure [1]. Superimposed on quadrupole deformed shapes, octupole $(\lambda=3)$ and hexadecapole $(\lambda=4)$ deformations are frequently considered as well, usually in terms of vibrational oscillations although there is evidence for nuclei with a permanent octupole deformation [2].

The accepted paradigm is that the spherical symmetry of the nucleus is reduced to a lower one which in most cases corresponds to a shape with a single axis of symmetry. In technical terms the spherical $\mathrm{SO}(3)$ symmetry is spontaneously broken and reduced to $\mathrm{SO}(2)$. Both $\mathrm{SO}(3)$ and $\mathrm{SO}(2)$ are examples of symmetries that depend on continuous variables, e.g., the three Euler angles or the angle of rotation around the axis of symmetry. Nothing prohibits
the further reduction of the symmetry of the intrinsic shape of the nucleus until a discrete (or point) symmetry with a finite number of invariance operations remains or even until no symmetry remains. A well-known possibility is quadrupole deformation with three axes of different length. The intrinsic nuclear shape in that case has no continuous symmetry but is invariant under the eight transformations that form the discrete group $\mathrm{D}_{2 \mathrm{~h}}$. (For a discussion of discrete groups see, e.g., Hamermesh [3].) The invariance of the nuclear shape under rotations and reflections - or the absence thereof in the case of deformation-determines the energy spectrum and leads to predictions that can be tested experimentally.

In 1994 Li and Dudek [4] pointed out that intrinsic shapes with a higher-rank discrete symmetry can be obtained in the context of the collective model and that, specifically, an octupole deformation with non-zero $\mu=2$ component (and all other multipoles zero) exhibits the tetrahedral symmetry $\mathrm{T}_{\mathrm{d}}$. In subsequent studies [5-8] this observation was followed up systematically and it was shown how the tetrahedral, octahedral and icosahedral discrete symmetries, $\mathrm{T}_{\mathrm{d}}, \mathrm{O}_{\mathrm{h}}$ and $\mathrm{I}_{\mathrm{h}}$, arise through combinations of deformations of specific multipolarity.

For a fermionic quantum system, e.g., an odd-mass nucleus or a single-particle nuclear Hamiltonian, time-reversal invariance must be considered as well. Due to Kramers' theorem, stationary eigenstates of such systems are at least twofold degenerate [9]. Inclusion of the operation of time reversal into the higher-rank discrete symmetries considered above leads to the enlarged versions $\mathrm{T}_{\mathrm{d}}^{\mathrm{D}}, \mathrm{O}_{\mathrm{h}}^{\mathrm{D}}$ and $\mathrm{I}_{\mathrm{h}}^{\mathrm{D}}$ (see $\S 99$ in Landau and Lifchitz [10] who denote these enlarged discrete groups with a prime). A prominent consequence of discrete symmetries of higher rank is the occurrence of more than twofold degenerate states in the spectrum of a single-particle nuclear Hamiltonian [4].

While the formal possibility of nuclear shapes with higher-rank discrete symmetries is by now well established, the question remains whether such exotic deformations are realized in nuclei. Over the years this question has been studied from a theoretical [11-13] and an experimental $[14,15]$ point of view. The former studies have been consistently carried out in a mean-field approach usually supplemented with pairing correlations. Concerning the experimental studies, it is fair to say that up to now no conclusive evidence has been found that unambiguously establishes the existence of a nucleus with a higher-rank discrete symmetry. A notable example is the study of Jentschel et al. [16] who failed to find a vanishing quadrupole moment of a negative-parity band in ${ }^{156} \mathrm{Gd}$ which should have been the 'smoking gun' of tetrahedral deformation.

On the other hand, discrete symmetries are rather well established in light nuclei in connection with alpha-particle clustering which itself has a long history in nuclear physics [17]. Algebraic models have been developed by Bijker
and Iachello $[18,19]$ with the aim to describe the discrete symmetries $D_{3 h}$ and $\mathrm{T}_{\mathrm{d}}$ associated with alpha-particles in a triangular or tetrahedral configuration. This approach has attracted renewed interest in view of novel experimental evidence recently found in ${ }^{12} \mathrm{C}$ and ${ }^{16} \mathrm{O}[20,21]$. Discrete symmetries associated with alpha-particle clustering, while an important and attractive field of activity, differ from those considered here where they arise in the context of the collective model of the nucleus.

The aim of this series of papers is to analyze the question of the possible occurrence of higher-rank discrete symmetries in nuclei from a different theoretical perspective. Since the work of Arima and Iachello [22] it is known that an alternative description of collective states in nuclei exists in terms of bosons in the context of the interacting boson model (IBM). Quadrupole collective states require $s$ and $d$ bosons, with angular momentum $\ell=0$ and $\ell=2$, respectively, and lead to the most elementary version of the model, the $s d$-IBM. Many refinements of this original version are possible [23] and already in the early papers on the IBM an $f$ boson $(\ell=3)$ is added to deal with negative-parity states with octupole collectivity [24-26]. Hexadecapole states, on the other hand, require the consideration of a $g$ boson with $\ell=4$.

It will be shown that the higher-rank discrete symmetries, as encountered in mean-field approaches, can also be realized in the context of an algebraic model with the relevant degrees of freedom and that, for example, tetrahedral and octahedral symmetries can be studied in the context of the $s f$-IBM and $s g$-IBM, respectively. Due to the pervasiveness of quadrupole collectivity in nuclei, the addition of a $d$ boson will make these algebraic models less schematic, leading to the $s d f$-IBM and $s d g$-IBM, respectively. (In the former case it might even be necessary to consider the $s p d f$-IBM with an additional negative-parity $p$ boson with $\ell=1[27]$.)

This series starts with an investigation of octahedral symmetries in the framework of the $s d g$-IBM, adopting the model's most general Hamiltonian with up to two-body interactions. The collective parameters of quadrupole and hexadecapole deformation and their relation to octahedral symmetry are recalled in Sect. 2. In Sect. 3 the general Hamiltonian of the $s d g$-IBM is defined and its corresponding classical limit in the most general coherent state is derived. The catastrophe analysis of the resulting energy surface is carried out in Sect. 4 with particular attention to the occurrence of minima with octahedral symmetry. First conclusions from this analysis are drawn in Sect. 5 .

## 2 Quadrupole and hexadecapole shapes

Shapes with octahedral discrete symmetry occur in lowest order through a combination of hexadecapole deformations $Y_{4 \mu}(\theta, \phi)$ with different $\mu$. To make the shape more realistic for nuclei, a quadrupole deformation should be added since that deformation is of lowest order in the geometric model of Bohr. With both these deformations the nuclear surface is parameterized in the following way:

$$
\begin{align*}
R(\theta, \phi)=R_{0}\left(1+a_{20} Y_{20}(\theta, \phi)\right. & +a_{22}\left[Y_{2-2}(\theta, \phi)+Y_{2+2}(\theta, \phi)\right] \\
+a_{40} Y_{40}(\theta, \phi) & +a_{42}\left[Y_{4-2}(\theta, \phi)+Y_{4+2}(\theta, \phi)\right] \\
& \left.+a_{44}\left[Y_{4-4}(\theta, \phi)+Y_{4+4}(\theta, \phi)\right]\right) . \tag{1}
\end{align*}
$$

It is customary to define quadrupole-deformation variables through

$$
\begin{equation*}
a_{20}=\beta_{2} \cos \gamma_{2}, \quad a_{22}=\sqrt{\frac{1}{2}} \beta_{2} \sin \gamma_{2}, \tag{2}
\end{equation*}
$$

where $\beta_{2}$ quantifies the quadrupole deviation from a sphere and $\gamma_{2}$ the deviation from a quadrupole shape with axial symmetry. Similarly, a hexadecapole variable $\beta_{4}$ is introduced which quantifies the deviation from a sphere. For the parameterization of hexadecapole asymmetric shapes two approaches have been adopted. In the first, a single $\gamma$ is introduced which parameterizes the deviation from axial symmetry at once for the quadrupole and hexadecapole degrees of freedom [28]. A symmetry argument then leads to a simplified parameterization in terms of three variables $\beta_{2}, \beta_{4}$ and $\gamma$,

$$
\begin{equation*}
a_{40}=\sqrt{\frac{1}{6}} \beta_{4}\left(5 \cos ^{2} \gamma+1\right), \quad a_{42}=\sqrt{\frac{15}{72}} \beta_{4} \sin 2 \gamma, \quad a_{44}=\sqrt{\frac{35}{72}} \beta_{4} \sin ^{2} \gamma \tag{3}
\end{equation*}
$$

In fact, there are three different such parameterizations [28] but Eq. (3) is the one that has been used up to now in the analysis of the $s d g$-IBM (see below). The parameter ranges are $0 \leq \beta_{2}<+\infty,-\infty<\beta_{4}<+\infty$ and $0 \leq \gamma \leq \pi / 3$, and the values $\gamma=0$ and $\gamma=\pi / 3$ lead to a shape with axial symmetry.

In a second approach, developed by Rohoziński and Sobiczewski [29], a separate, independent asymmetry parameter $\gamma_{4}$ is introduced for the hexadecapole deformation. Furthermore, to describe the full range of possible hexadecapole deformations, an additional variable $\delta_{4}$ is needed, which represents the convexity or concavity of the shape. This leads to five shape variables, two quadrupole and three hexadecapole ones which are related as follows to the original parameterization (1):

$$
\begin{align*}
& a_{40}=\beta_{4}\left(\sqrt{\frac{7}{12}} \cos \delta_{4}+\sqrt{\frac{5}{12}} \sin \delta_{4} \cos \gamma_{4}\right), \\
& a_{42}=-\sqrt{\frac{1}{2}} \beta_{4} \sin \delta_{4} \sin \gamma_{4}, \\
& a_{44}=\beta_{4}\left(\sqrt{\frac{5}{24}} \cos \delta_{4}-\sqrt{\frac{7}{24}} \sin \delta_{4} \cos \gamma_{4}\right), \tag{4}
\end{align*}
$$

where the parameter ranges are now $0 \leq \beta_{4}<+\infty, 0 \leq \gamma_{4} \leq \pi / 3$ and $0 \leq \delta_{4} \leq \pi$. An axially symmetric shape occurs for $a_{42}=a_{44}=0$. This corresponds to $\gamma_{4}=0$ and $\delta_{4}=\arccos \sqrt{7 / 12}$.

A shape with octahedral symmetry implies a vanishing quadrupole deformation, $a_{20}=a_{22}=0$, and can be realized in lowest order with a hexadecapole deformation that satisfies $[6,30]$

$$
\begin{equation*}
a_{42}=0, \quad a_{44} / a_{40}= \pm \sqrt{5 / 14} \tag{5}
\end{equation*}
$$

The nuclear surface (1) then reduces to

$$
\begin{equation*}
R(\theta, \phi)=R_{0}\left(1+a_{40}\left[Y_{40}(\theta, \phi) \pm \sqrt{\frac{5}{14}}\left[Y_{4-4}(\theta, \phi)+Y_{4+4}(\theta, \phi)\right]\right]\right) . \tag{6}
\end{equation*}
$$

Such shapes cannot be generated with the restricted parameterization (3), which therefore is insufficient for the present purpose. For positive values of $a_{40}$ an octahedron is obtained while for negative $a_{40}$ one finds a cube, the dual of the octahedron, both shapes having octahedral symmetry. The sign of the ratio $a_{44} / a_{40}$ does not affect the intrinsic shape; the opposite sign corresponds to the same shape rotated over $\pi / 2$ around the $z$ axis. The four different cases are illustrated in Fig. 1.

In the parameterization (4) the first of the octahedral conditions (5) implies $\delta_{4}=0, \delta_{4}=\pi$ or $\gamma_{4}=0$. For $\delta_{4}=0$ or $\delta_{4}=\pi$, the second of the octahedral conditions (5) is automatically satisfied for any value of $\gamma_{4}$, resulting in a positive ratio $a_{44} / a_{40}$; if $\delta_{4}=0$, the shape is an octahedron while for $\delta_{4}=$ $\pi$ it is a cube. For the remaining case of $\gamma_{4}=0$ one finds an additional solution with octahedral symmetry for $\delta_{4}=\arccos (1 / 6)$, corresponding to a rotated octahedron, see Fig. 1c, but no rotated cube can be obtained with the parameterization (4).

In the quadrupole parameterization (2) a given couple $\left(\beta_{2}, \gamma_{2}\right)$ with $\beta_{2} \in$ $\left[0,+\infty\left[\right.\right.$ and $\gamma_{2} \in[0, \pi / 3]$ corresponds to a unique intrinsic shape. This is not the case for the hexadecapole parameterization (4), that is, different triplets $\left(\beta_{4}, \delta_{4}, \gamma_{4}\right)$ with $\beta_{4} \in\left[0,+\infty\left[, \delta_{4} \in[0, \pi]\right.\right.$ and $\gamma_{4} \in[0, \pi / 3]$ may lead to the same intrinsic shape, differently oriented with respect to the laboratory frame. An example of the latter are the triplets $\left(\beta_{4}, \delta_{4}=0, \gamma_{4}=\right.$ anything $)$ and $\left(\beta_{4}, \delta_{4}=\arccos (1 / 6), \gamma_{4}=0\right)$ which correspond to the same intrinsic shape


Fig. 1. Hexadecapole deformed surfaces with octahedral symmetry. Four cases are shown: (a) and (c) are octahedrons with $a_{40}=0.2$; (b) and (d) are cubes with $a_{40}=-0.2$. Octahedral symmetry is obtained for $a_{42}=0$ and $a_{44} / a_{40}=+\sqrt{5 / 14}$ [(a) and (b)], or $a_{42}=0$ and $a_{44} / a_{40}=-\sqrt{5 / 14}[(\mathrm{c})$ and (d)]. The two signs of $a_{44} / a_{40}$ correspond to the same intrinsic shape but rotated over $\pi / 2$ around the $z$ axis. In terms of the parameters in Eq. (4): (a) $\beta_{4}=0.2$ and $\delta_{4}=0$, (b) $\beta_{4}=0.2$ and $\delta_{4}=\pi$, (c) $\beta_{4}=0.2, \delta_{4}=\arccos (1 / 6)$ and $\gamma_{4}=0$, (d) not possible.
for any value of $\beta_{4}$. Shapes that are intrinsically the same lead to identical conditions on the interaction parameters in the Hamiltonian, as will be shown below.

## 3 The $s d g$ interacting boson model

Since the bosons of the IBM represent pairs of valence nucleons, a nucleus is characterized by a constant total number of bosons $N$ which equals half the number of valence nucleons. An important feature of the $s d$-IBM is the existence of a $U(6)$ dynamical algebra, the substructure of which leads to analytically solvable limits, also called dynamical symmetries. The sd-IBM can successfully describe quadrupole collective states in even-even nuclei but other
features require an extension of the $s d$-IBM. In particular, the hexadecapole degree of freedom requires the introduction of a $g$ boson $(\ell=4)$ and the upgrade of the dynamical algebra from $U(6)$ to $U(15)$. We do not cite here the many papers related to the $s d g$-IBM but refer the reader to the excellent review by Devi and Kota [31].

### 3.1 Hamiltonian of the sdg-IBM

Since the Hamiltonian of the $s d g$-IBM conserves the total number of bosons, it can be written in terms of the 225 operators $b_{\ell m}^{\dagger} b_{\ell^{\prime} m^{\prime}}$ where $b_{\ell m}^{\dagger}\left(b_{\ell m}\right)$ creates (annihilates) a boson with angular momentum $\ell$ and $z$ projection $m$. This set of 225 operators generates the Lie algebra $\mathrm{U}(15)$. A boson-number-conserving Hamiltonian with up to two-body interactions is of the form

$$
\begin{equation*}
\hat{H}=\hat{H}_{1}+\hat{H}_{2} \tag{7}
\end{equation*}
$$

The first term is the one-body part

$$
\begin{align*}
\hat{H}_{1} & =\epsilon_{s}\left[s^{\dagger} \times \tilde{s}\right]^{(0)}+\epsilon_{d} \sqrt{5}\left[d^{\dagger} \times \tilde{d}\right]^{(0)}+\epsilon_{g} \sqrt{9}\left[g^{\dagger} \times \tilde{g}\right]^{(0)} \\
& \equiv \epsilon_{s} s^{\dagger} \cdot \tilde{s}+\epsilon_{d} d^{\dagger} \cdot \tilde{d}+\epsilon_{g} g^{\dagger} \cdot \tilde{g} \\
& \equiv \epsilon_{s} \hat{n}_{s}+\epsilon_{d} \hat{n}_{d}+\epsilon_{g} \hat{n}_{g}, \tag{8}
\end{align*}
$$

where the multiplication $\times$ refers to coupling in angular momentum (shown as an upperscript in round brackets), the dot • indicates a scalar product and $\tilde{b}_{\ell m} \equiv(-)^{\ell-m} b_{\ell,-m}$. Furthermore, $\hat{n}_{\ell}$ is the number operator for the $\ell$ boson and the coefficient $\epsilon_{\ell}$ is its energy. The second term in the Hamiltonian (7) represents the two-body interaction

$$
\begin{equation*}
\hat{H}_{2}=\sum_{\ell_{1} \leq \ell_{2}, \ell_{1}^{\prime} \leq \ell_{2}^{\prime}, L} \frac{(-)^{L} v_{\ell_{1} \ell_{2} \ell_{1}^{\prime} \ell_{2}^{\prime}}^{L}}{\sqrt{\left(1+\delta_{\ell_{1} \ell_{2}}\right)\left(1+\delta_{\ell_{1}^{\prime} \ell_{2}^{\prime}}\right)}}\left[b_{\ell_{1}}^{\dagger} \times b_{\ell_{2}}^{\dagger}\right]^{(L)} \cdot\left[\tilde{b}_{\ell_{2}^{\prime}} \times \tilde{b}_{\ell_{1}^{\prime}}\right]^{(L)}, \tag{9}
\end{equation*}
$$

where the coefficients $v_{\ell_{1} \ell_{2} \ell_{1}^{\prime} \ell_{2}^{\prime}}^{L}$ are the interaction matrix elements between normalized two-boson states,

$$
\begin{equation*}
v_{\ell_{1} \ell_{2} \ell_{1}^{\prime} \ell_{2}^{\prime}}^{L}=\left\langle\ell_{1} \ell_{2} ; L M_{L}\right| \hat{H}_{2}\left|\ell_{1}^{\prime} \ell_{2}^{\prime} ; L M_{L}\right\rangle \tag{10}
\end{equation*}
$$

It is henceforth assumed that $\ell_{1} \leq \ell_{2}$ and $\ell_{1}^{\prime} \leq \ell_{2}^{\prime}$.
Once the single-boson energies $\epsilon_{\ell}$ and interaction matrix elements $v_{\ell_{1} \ell_{2} \ell_{1}^{\prime} 1_{2}^{\prime}}^{L}$ are known, the most general two-body $s d g$-Hamiltonian is uniquely determined.

### 3.2 Classical limit of the sdg-IBM

The classical limit of any boson Hamiltonian is defined as its expectation value in a coherent state [32]. This yields a function of the deformation variables which can be interpreted as a total energy surface depending on these variables. The method was first proposed for the $s d$-IBM [33,34]. The extension to the $s d g$-IBM was carried out by Devi and Kota [35] for the simplified parameterization (3).

The generic form of the coherent state for the $s d g$-IBM is

$$
\begin{equation*}
\left|N ; a_{2 \mu}, a_{4 \mu}\right\rangle \propto \Gamma\left(a_{2 \mu}, a_{4 \mu}\right)^{N}|\mathrm{o}\rangle \tag{11}
\end{equation*}
$$

where

$$
\begin{equation*}
\Gamma\left(a_{2 \mu}, a_{4 \mu}\right)=s^{\dagger}+\sum_{\mu=0,2} a_{2 \mu}\left(d_{-\mu}^{\dagger}+d_{+\mu}^{\dagger}\right)+\sum_{\mu=0,2,4} a_{4 \mu}\left(g_{-\mu}^{\dagger}+g_{+\mu}^{\dagger}\right) \tag{12}
\end{equation*}
$$

and $|0\rangle$ is the boson vacuum. The $a_{\lambda \mu}$ have the interpretation of shape variables appearing in the expansion (1). Since the deformation in the IBM is generated by the valence nucleons only, in contrast to the geometric model of Bohr and Mottelson [1] where it is associated with the entire nucleus, the shape variables in both models are proportional but not identical [36]. In terms of the variables in the parameterizations (2), (3) and (4), $\beta_{2}$ and $\beta_{4}$ are proportional in both models while the angles $\gamma$ or $\gamma_{2}, \gamma_{4}$ and $\delta_{4}$ have an identical interpretation.

The coherent state based on the parameterization (3)

$$
\begin{equation*}
\left|N ; \beta_{2}, \beta_{4}, \gamma\right\rangle=\sqrt{\frac{1}{N!\left(1+\beta_{2}^{2}+\beta_{4}^{2}\right)^{N}}} \Gamma\left(\beta_{2}, \beta_{4}, \gamma\right)^{N}|\mathrm{o}\rangle \tag{13}
\end{equation*}
$$

with

$$
\begin{align*}
\Gamma\left(\beta_{2}, \beta_{4}, \gamma\right)= & s^{\dagger}+\beta_{2}\left[\cos \gamma d_{0}^{\dagger}+\sqrt{\frac{1}{2}} \sin \gamma\left(d_{-2}^{\dagger}+d_{+2}^{\dagger}\right)\right] \\
& +\beta_{4}\left[\frac{1}{6}\left(5 \cos ^{2} \gamma+1\right) g_{0}^{\dagger}+\sqrt{\frac{15}{72}} \sin 2 \gamma\left(g_{-2}^{\dagger}+g_{+2}^{\dagger}\right)\right. \\
& \left.+\sqrt{\frac{35}{72}} \sin ^{2} \gamma\left(g_{-4}^{\dagger}+g_{+4}^{\dagger}\right)\right] \tag{14}
\end{align*}
$$

was used by Devi and Kota [35] to derive the geometry of the different limits of the $s d g$-IBM. The expression for the classical limit of the general $s d g$-Hamiltonian (7) with this coherent state was given in Ref. [37].

If one is interested in octahedral shapes and how they appear in the $s d g$-IBM, the general parameterization (4) is needed, and the appropriate coherent state is

$$
\begin{equation*}
\left|N ; \beta_{2}, \beta_{4}, \gamma_{2}, \gamma_{4}, \delta_{4}\right\rangle=\sqrt{\frac{1}{N!\left(1+\beta_{2}^{2}+\beta_{4}^{2}\right)^{N}}} \Gamma\left(\beta_{2}, \beta_{4}, \gamma_{2}, \gamma_{4}, \delta_{4}\right)^{N}|\mathrm{o}\rangle, \tag{15}
\end{equation*}
$$

with

$$
\begin{align*}
\Gamma\left(\beta_{2}, \beta_{4}, \gamma_{2}, \gamma_{4}, \delta_{4}\right)=s^{\dagger}+ & \beta_{2}\left[\cos \gamma_{2} d_{0}^{\dagger}+\sqrt{\frac{1}{2}} \sin \gamma_{2}\left(d_{-2}^{\dagger}+d_{+2}^{\dagger}\right)\right]  \tag{16}\\
+\beta_{4}[ & \left(\sqrt{\frac{7}{12}} \cos \delta_{4}+\sqrt{\frac{5}{12}} \sin \delta_{4} \cos \gamma_{4}\right) g_{0}^{\dagger} \\
& \quad-\sqrt{\frac{1}{2}} \sin \delta_{4} \sin \gamma_{4}\left(g_{-2}^{\dagger}+g_{+2}^{\dagger}\right) \\
& \left.+\left(\sqrt{\frac{5}{24}} \cos \delta_{4}-\sqrt{\frac{7}{24}} \sin \delta_{4} \cos \gamma_{4}\right)\left(g_{-4}^{\dagger}+g_{+4}^{\dagger}\right)\right]
\end{align*}
$$

The classical limit of any Hamiltonian of the $s d g$-IBM is, for the general coherent state (15), defined as

$$
\begin{equation*}
\langle\hat{H}\rangle \equiv\left\langle N ; \beta_{2}, \beta_{4}, \gamma_{2}, \gamma_{4}, \delta_{4}\right| \hat{H}\left|N ; \beta_{2}, \beta_{4}, \gamma_{2}, \gamma_{4}, \delta_{4}\right\rangle . \tag{17}
\end{equation*}
$$

Once the form of the coherent state has been determined, the expectation value (17) can be obtained with the method of differentiation [38] which lends itself ideally to programming in a symbolic language. The classical limit of the one-body part (8) is

$$
\begin{equation*}
\left\langle\hat{H}_{1}\right\rangle=N \frac{\epsilon_{s}+\epsilon_{d} \beta_{2}^{2}+\epsilon_{g} \beta_{4}^{2}}{1+\beta_{2}^{2}+\beta_{4}^{2}} \tag{18}
\end{equation*}
$$

while that of its two-body part (9) can be written in the generic form

$$
\begin{equation*}
\left\langle\hat{H}_{2}\right\rangle=\frac{N(N-1)}{\left(1+\beta_{2}^{2}+\beta_{4}^{2}\right)^{2}} \sum_{k l} \beta_{2}^{k} \beta_{4}^{l}\left[c_{k l}+\sum_{i j} c_{k l}^{i j} \cos \left(i \gamma_{2}+j \gamma_{4}\right) \phi_{k l}^{i j}\left(\delta_{4}\right)\right] \tag{19}
\end{equation*}
$$

where the coefficients $c_{k l}$ and $c_{k l}^{i j}$ can be expressed in terms of the interactions $v_{\ell_{1} \ell_{2} \ell_{1}^{\prime} \ell_{2}^{\prime}}^{L}$. The expressions for the non-zero coefficients $c_{k l}$ are

$$
\begin{aligned}
& c_{00}=\frac{1}{2} v_{s s s s}^{0}, \quad c_{20}=\sqrt{\frac{1}{5}} v_{s s \cdot d d}^{0}+v_{s d s d}^{2}, \quad c_{02}=\frac{1}{3} v_{s s \cdot g g}^{0}+v_{s g s g}^{4}, \\
& c_{40}=\frac{1}{10} v_{d d d d}^{0}+\frac{1}{7} v_{d d d}^{2}+\frac{9}{35} v_{d d d d}^{4}, \\
& c_{22}=\frac{1}{3 \sqrt{5}} v_{d d \cdot g g}^{0}+\frac{7}{\sqrt{715}} v_{d d \cdot g g}^{4}+\frac{1}{6} v_{d g d g}^{2}+\frac{4}{11} v_{d g d g}^{4}+\frac{1}{6} v_{d g d g}^{5}+\frac{10}{33} v_{d g d g}^{6},
\end{aligned}
$$

$$
\begin{equation*}
c_{04}=\frac{1}{18} v_{g g g g}^{0}+\frac{38}{693} v_{g g g g}^{2}+\frac{89}{1001} v_{g g g g}^{4}+\frac{62}{495} v_{g g g g}^{6}+\frac{1129}{6435} v_{g g g g}^{8}, \tag{20}
\end{equation*}
$$

while those for the non-zero coefficients $c_{k l}^{i j}$ are

$$
\begin{align*}
& c_{30}^{30}=-\frac{2}{\sqrt{7}} v_{s d \cdot d d}^{2}, \\
& c_{21}^{00}= \sqrt{\frac{2}{3}} v_{s d \cdot d g}^{2}+\sqrt{\frac{3}{5}} v_{s g \cdot d d}^{4}, \quad c_{21}^{21}=\sqrt{\frac{10}{21}} v_{s d \cdot d g}^{2}+\sqrt{\frac{3}{7}} v_{s g \cdot d d}^{4}, \\
& c_{12}^{1-1}=-\frac{2}{3} \sqrt{\frac{10}{11}} v_{s d \cdot g g}^{2}-\frac{4}{\sqrt{11}} v_{s g \cdot d g}^{4}, \quad c_{12}^{12}=\frac{2}{3} \sqrt{\frac{2}{77}} v_{s d \cdot g g}^{2}+\frac{4}{\sqrt{385}} v_{s g \cdot d g}^{4}, \\
& c_{03}^{00}= \frac{2}{\sqrt{429}} v_{s g \cdot g g}^{4}, \quad c_{03}^{03}=\sqrt{\frac{80}{3003}} v_{s g \cdot g g}^{4}, \\
& c_{31}^{1-1}=-\frac{1}{7} \sqrt{\frac{10}{3}} v_{d d \cdot d g}^{2}-\frac{2}{7} \sqrt{\frac{15}{11}} v_{d d \cdot d g}^{4}, \quad c_{31}^{30}=-\sqrt{\frac{2}{21}} v_{d d \cdot d g}^{2}-\sqrt{\frac{12}{77}} v_{d d \cdot d g}^{4}, \\
& c_{22}^{00}=-\frac{3}{\sqrt{715}} v_{d d \cdot g g}^{4}-\frac{1}{42} v_{d g d g}^{2}+\frac{1}{15} v_{d g d g}^{3}-\frac{27}{385} v_{d g d g}^{4}+\frac{1}{30} v_{d g d g}^{5}-\frac{1}{165} v_{d g d g}^{6}, \\
& c_{22}^{2-2}=-\frac{2}{21} \sqrt{\frac{2}{11}} v_{d d \cdot g g}^{2}+\frac{4}{7} \sqrt{\frac{5}{143}} v_{d d \cdot g g}^{4}-\frac{1}{15} v_{d g d g}^{3}+\frac{1}{11} v_{d g d g}^{4}-\frac{4}{165} v_{d g d g}^{6}, \\
& c_{22}^{21}= \frac{2}{3} \sqrt{\frac{10}{77}} v_{d d \cdot g g}^{2}+\sqrt{\frac{1}{1001}} v_{d d \cdot g g}^{4}+\frac{1}{6} \sqrt{\frac{5}{7}} v_{d g d g}^{2}-\frac{8}{11 \sqrt{35}} v_{d g d g}^{4}-\frac{1}{6} \sqrt{\frac{7}{5}} v_{d g d g}^{5} \\
&+\frac{\sqrt{35}}{33} v_{d g d g}^{6}, \\
& c_{13}^{1-1}=-\frac{4}{21} \sqrt{\frac{5}{33}} v_{d g \cdot g g}^{2}-\frac{12}{77} \sqrt{\frac{3}{13}} v_{d g \cdot g g}^{4}-\frac{2}{33} \sqrt{\frac{10}{3}} v_{d g \cdot g g}^{6} \\
& c_{13}^{12}=-\frac{4}{3 \sqrt{231}} v_{d g \cdot g g}^{2}-\frac{12}{11} \sqrt{\frac{3}{455}} v_{d g \cdot g g}^{4}-\frac{2}{33} \sqrt{\frac{14}{3}} v_{d g \cdot g g}^{6} \\
& c_{04}^{00}=-\frac{2}{693} v_{g g g g}^{2}+\frac{4}{3003} v_{g g g g}^{4}+\frac{2}{495} v_{g g g g}^{6}-\frac{16}{6435} v_{g g g g}^{8}, \\
& c_{04}^{03}=-\frac{2}{99} \sqrt{\frac{5}{7}} v_{g g g g}^{2}+\frac{4}{429} \sqrt{\frac{5}{7}} v_{g g g g}^{4}+\frac{2}{99} \sqrt{\frac{7}{5}} v_{g g g g}^{6}-\frac{16}{1287} \sqrt{\frac{7}{5}} v_{g g g g}^{8}, \tag{21}
\end{align*}
$$

where the notation $v_{\ell_{1} \ell_{2} \cdot \ell_{1}^{\prime} \ell_{2}^{\prime}}^{L} \equiv v_{\ell_{1} \ell_{2} \ell_{1}^{\prime} \ell_{2}^{\prime}}^{L}+v_{\ell_{1}^{\prime} \ell_{2}^{\prime} \ell_{1} \ell_{2}}^{L}$ is introduced for $\left(\ell_{1} \ell_{2}\right) \neq$ $\left(\ell_{1}^{\prime} \ell_{2}^{\prime}\right)$ since this combination consistently occurs due to the hermiticity of the Hamiltonian. Furthermore, the $\phi_{k l}^{i j}\left(\delta_{4}\right)$ are functions defined as follows:

$$
\begin{align*}
& \phi_{30}^{30}\left(\delta_{4}\right)=1, \quad \phi_{21}^{00}\left(\delta_{4}\right)=\cos \delta_{4}, \quad \phi_{21}^{21}\left(\delta_{4}\right)=\sin \delta_{4} \\
& \phi_{12}^{1-1}\left(\delta_{4}\right)=\sin 2 \delta_{4}, \quad \phi_{12}^{12}\left(\delta_{4}\right)=1-\cos 2 \delta_{4} \\
& \phi_{03}^{00}\left(\delta_{4}\right)=6 \cos \delta_{4}+\cos 3 \delta_{4}, \quad \phi_{03}^{03}\left(\delta_{4}\right)=3 \sin \delta_{4}-\sin 3 \delta_{4} \\
& \phi_{31}^{1-1}\left(\delta_{4}\right)=\sin \delta_{4}, \quad \phi_{31}^{30}\left(\delta_{4}\right)=\cos \delta_{4} \\
& \phi_{22}^{00}\left(\delta_{4}\right)=\phi_{22}^{2-2}\left(\delta_{4}\right)=1-\cos 2 \delta_{4}, \quad \phi_{22}^{21}\left(\delta_{4}\right)=\sin 2 \delta_{4} \\
& \phi_{13}^{1-1}\left(\delta_{4}\right)=\sin \delta_{4}+2 \sin 3 \delta_{4}, \quad \phi_{13}^{12}\left(\delta_{4}\right)=\cos \delta_{4}-\cos 3 \delta_{4} \\
& \phi_{04}^{00}\left(\delta_{4}\right)=2 \cos 2 \delta_{4}+17 \cos 4 \delta_{4}, \quad \phi_{04}^{03}\left(\delta_{4}\right)=2 \sin 2 \delta_{4}-\sin 4 \delta_{4} \tag{22}
\end{align*}
$$

These functions can be written concisely as

$$
\begin{equation*}
\phi_{k l}^{i j}\left(\delta_{4}\right)=\sum_{n=l, l-2, \ldots}^{0 \text { or } 1} c_{k l n}^{i j} \varphi_{j}\left(n \delta_{4}\right) \tag{23}
\end{equation*}
$$

where $\varphi_{j}(\theta)$ is $\cos \theta(\sin \theta)$ for even (odd) $j$, with the following interaction-
independent constants:

$$
\begin{array}{ll}
c_{300}^{30}=1, & c_{211}^{00}=1, \quad c_{211}^{21}=1, \\
c_{120}^{1-1}=0, & c_{122}^{1-1}=1, \quad c_{120}^{12}=1, \quad c_{122}^{12}=-1, \\
c_{031}^{00}=6, & c_{033}^{00}=1, \quad c_{031}^{03}=3, \quad c_{033}^{03}=-1, \\
c_{31}^{1-1}=1, & c_{311}^{30}=1, \\
c_{220}^{00}=c_{220}^{2-2}=1, \quad c_{222}^{00}=c_{22}^{2-2}=-1, \quad c_{220}^{21}=0, \quad c_{222}^{21}=1, \\
c_{131}^{1-1}=1, & c_{133}^{1-1}=2, \quad c_{131}^{12}=1, \quad c_{133}^{12}=-1, \\
c_{040}^{00}=0, & c_{042}^{00}=2, \quad c_{044}^{00}=17, \quad c_{040}^{03}=0, \quad c_{042}^{03}=2, \quad c_{044}^{03}=-1 . \tag{24}
\end{array}
$$

The classical limit of the total Hamiltonian (7) can therefore be written as

$$
\begin{align*}
\langle\hat{H}\rangle & \equiv E\left(\beta_{2}, \beta_{4}, \gamma_{2}, \gamma_{4}, \delta_{4}\right) \\
& =\frac{N(N-1)}{\left(1+\beta_{2}^{2}+\beta_{4}^{2}\right)^{2}} \sum_{k l} \beta_{2}^{k} \beta_{4}^{l}\left[c_{k l}^{\prime}+\sum_{i j} c_{k l}^{i j} \cos \left(i \gamma_{2}+j \gamma_{4}\right) \phi_{k l}^{i j}\left(\delta_{4}\right)\right] \tag{25}
\end{align*}
$$

where $c_{k l}^{\prime}$ are the modified coefficients

$$
\begin{array}{ll}
c_{00}^{\prime}=c_{00}+\epsilon_{s}^{\prime}, & c_{20}^{\prime}=c_{20}+\epsilon_{s}^{\prime}+\epsilon_{d}^{\prime}, \\
c_{40}^{\prime}=c_{40}+\epsilon_{d}^{\prime}, & c_{22}^{\prime}=c_{22}+\epsilon_{d}^{\prime}+\epsilon_{g}^{\prime},  \tag{26}\\
c_{04}^{\prime}=\epsilon_{04}^{\prime}+\epsilon_{g}^{\prime},
\end{array}
$$

in terms of the scaled boson energies $\epsilon_{\ell}^{\prime} \equiv \epsilon_{\ell} /(N-1)$. While the differentiation technique [38] allows a secure derivation of the expectation value (17), the particular representation (25) in terms of functions $\beta_{2}^{k} \beta_{4}^{l} \cos \left(i \gamma_{2}+j \gamma_{4}\right) \phi_{k l}^{i j}\left(\delta_{4}\right)$ is not obtained automatically. The correctness of the latter representation can be proven by use of trigonometric conversion algorithms which show it to be identical to the expression found with the brute-force differentiation technique.

The quantum-mechanical Hamiltonian (7), if it is hermitian, depends on three single-boson energies $\epsilon_{\ell}$ and 32 two-body interactions $v_{\ell_{1} \ell_{2} \ell_{1}^{\prime} \ell_{2}^{\prime}}^{L}$. In the classical limit with the most general coherent state (15), the number of independent parameters in the energy surface $E\left(\beta_{2}, \beta_{4}, \gamma_{2}, \gamma_{4}, \delta_{4}\right)$ is reduced to 22 (six coefficients $c_{k l}^{\prime}$ and 16 coefficients $\left.c_{k l}^{i j}\right)$. For comparison, if the simpler coherent state (13) is taken [37], this number is further reduced to 15.

## 4 Octahedral shapes in the $s d g$-IBM

### 4.1 Principle of the method

It is clear that a catastrophe analysis of the energy surface $E\left(\beta_{2}, \beta_{4}, \gamma_{2}, \gamma_{4}, \delta_{4}\right)$ with its five order parameters and 22 control parameters is beyond the scope of any reasonable analysis. Fortunately, this is not needed if one is interested in the realization of octahedral symmetry in the $s d g$-IBM. For this purpose one just wants to know what are the conditions on the interactions in the $s d g$-Hamiltonian for the surface (25) to have a minimum with octahedral symmetry. As shown in Sect. 2, a shape with such symmetry occurs for (i) $\beta_{2}=0, \beta_{4} \neq 0, \gamma_{2}=$ anything, $\gamma_{4}=$ anything and $\delta_{4}=0$, (ii) $\beta_{2}=0$, $\beta_{4} \neq 0, \gamma_{2}=$ anything, $\gamma_{4}=$ anything and $\delta_{4}=\pi$, or (iii) $\beta_{2}=0, \beta_{4} \neq 0$, $\gamma_{2}=$ anything, $\gamma_{4}=0$ and $\delta_{4}=\arccos (1 / 6)$.

The conditions for the energy surface $E\left(\beta_{2}, \beta_{4}, \gamma_{2}, \gamma_{4}, \delta_{4}\right)$ to have an extremum at $p^{*}$ are

$$
\begin{equation*}
\left.\frac{\partial E}{\partial \beta_{2}}\right|_{p^{*}}=\left.\frac{\partial E}{\partial \beta_{4}}\right|_{p^{*}}=\left.\frac{\partial E}{\partial \gamma_{2}}\right|_{p^{*}}=\left.\frac{\partial E}{\partial \gamma_{4}}\right|_{p^{*}}=\left.\frac{\partial E}{\partial \delta_{4}}\right|_{p^{*}}=0 \tag{27}
\end{equation*}
$$

where $p^{*} \equiv\left(\beta_{2}^{*}, \beta_{4}^{*}, \gamma_{2}^{*}, \gamma_{4}^{*}, \delta_{4}^{*}\right)$ is a short-hand notation for an arbitrary critical point. Furthermore, a critical point with octahedral symmetry shall be denoted as $o^{*}$ which implies that $o^{*}$ is one of the three cases (i), (ii) or (iii) listed above. While the Eqs. (27) are necessary for $E\left(\beta_{2}, \beta_{4}, \gamma_{2}, \gamma_{4}, \delta_{4}\right)$ to have an extremum at $p^{*}$, the conditions for a minimum require in addition that the eigenvalues of the stability matrix [i.e., the partial derivatives of $E\left(\beta_{2}, \beta_{4}, \gamma_{2}, \gamma_{4}, \delta_{4}\right)$ of second order] are all non-negative. All expressions in this section are obtained starting from the generic expression (25) for the energy surface and its derivatives up to second order.

### 4.2 Extrema with octahedral symmetry

Let us now apply the above procedure to the case of octahedral symmetry which requires the establishment of an extremum of the energy surface $E\left(\beta_{2}, \beta_{4}, \gamma_{2}, \gamma_{4}, \delta_{4}\right)$ for $p^{*}=o^{*}$.

Consider first the case of an octahedral shape (i) or a cubic shape (ii), cases that can be treated simultaneously. Four of the five extremum conditions (27) are identically satisfied for $p^{*}=o^{*}$ and do not lead to any constraints on the
coefficients $c_{k l}^{\prime}$ and $c_{k l}^{i j}$. The derivative in $\beta_{4}$ leads to the equation

$$
\begin{equation*}
\beta_{4}^{*}\left[-4 c_{00}^{\prime}+2 c_{02}^{\prime} \pm 21 c_{03}^{00} \beta_{4}^{*}-\left(2 c_{02}^{\prime}-4 c_{04}^{\prime}-76 c_{04}^{00}\right) \beta_{4}^{* 2} \mp 7 c_{03}^{00} \beta_{4}^{* 3}\right]=0, \tag{28}
\end{equation*}
$$

where the upper (lower) sign applies to $\delta_{4}^{*}=0\left(\delta_{4}^{*}=\pi\right)$. The spherical point $\beta_{4}^{*}=0$ is always an extremum of the energy surface. Other extrema $\beta_{4}^{*}$ are found as solutions of a cubic equation and therefore have cumbersome expressions. In the search for octahedral minima one is not interested in numerical values or analytic expressions for $\beta_{4}^{*}$ but one simply wants to know whether a hexadecapole deformed minimum exists or not. This question can be readily answered if one assumes the coefficients of the odd powers of $\beta_{4}^{*}$ in Eq. (28) to be zero, which happens for $c_{03}^{00}=0$. In that case, the non-zero solutions of Eq. (28) are

$$
\begin{equation*}
\beta_{4}^{*}= \pm \sqrt{\frac{2 c_{00}^{\prime}-c_{02}^{\prime}}{-c_{02}^{\prime}+2 c_{04}^{\prime}+38 c_{04}^{00}}}, \tag{29}
\end{equation*}
$$

leading to the conclusion that a real, positive $\beta_{4}^{*}$ is found if the combinations $2 c_{00}^{\prime}-c_{02}^{\prime}$ and $-c_{02}^{\prime}+2 c_{04}^{\prime}+38 c_{04}^{00}$ have the same sign. For non-zero values of $c_{03}^{00}$ [which is related to the $s$ - $g$ mixing matrix element $v_{s g \cdot g g}^{4}$, see Eq. (21)] the analysis is more complicated. The cubic equation (28) has real coefficients and therefore it always has at least one real solution $\beta_{4}^{*}$. In addition, since the ratio $\mp c_{03}^{00} /\left(-4 c_{00}^{\prime}+2 c_{02}^{\prime}\right)$ is negative for one of the choices $\delta_{4}^{*}=0$ or $\delta_{4}^{*}=\pi$, it follows that the solution $\beta_{4}^{*}$ is positive in that case. We conclude that there exists always an extremum with octahedral symmetry for any $s d g$-Hamiltonian except in the pathological case of no $s-g$ mixing, $v_{s g \cdot g g}^{4}=0$, in which case the condition is that the combinations $2 c_{00}^{\prime}-c_{02}^{\prime}$ and $-c_{02}^{\prime}+2 c_{04}^{\prime}+38 c_{04}^{00}$ should have the same sign.

For the case (iii) with $\delta_{4}=\arccos (1 / 6)$, the derivatives in $\gamma_{2}$ and $\gamma_{4}$ are identically zero and do not lead to any condition. The derivatives in $\beta_{2}, \beta_{4}$ and $\delta_{4}$ lead to the equations

$$
\begin{align*}
& \beta_{4}^{* 2}\left[-3\left(\sqrt{35} c_{12}^{1-1}+35 c_{12}^{12}\right)+7\left(\sqrt{35} c_{13}^{1-1}-5 c_{13}^{12}\right) \beta_{4}^{*}\right]=0, \\
& \beta_{4}^{*}\left[324\left(-2 c_{00}^{\prime}+c_{02}^{\prime}\right)+63\left(4 c_{03}^{00}+5 \sqrt{35} c_{03}^{03}\right) \beta_{4}^{*}\right. \\
& \quad+4\left(-81 c_{02}^{\prime}+162 c_{04}^{\prime}+1853 c_{04}^{00}+35 \sqrt{35} c_{04}^{03}\right) \beta_{4}^{* 2} \\
& \left.\quad-21\left(4 c_{03}^{00}+5 \sqrt{35} c_{03}^{03}\right) \beta_{4}^{* 3}\right]=0, \\
& \beta_{4}^{* 3}\left[9\left(-2 \sqrt{35} c_{03}^{00}+7 c_{03}^{03}\right)+224\left(\sqrt{35} c_{04}^{00}-c_{04}^{03}\right) \beta_{4}^{*}\right]=0 . \tag{30}
\end{align*}
$$

It would therefore seem that for the energy surface (25) the critical conditions in the case (iii) lead to equations that are different from the those obtained
in the cases (i) and (ii). It should not be forgotten, however, that the coefficients $c_{k l}^{\prime}$ and $c_{k l}^{i j}$ are expressed in terms of single-boson energies $\epsilon_{\ell}$ and interaction matrix elements $v_{\ell_{1} \ell_{2} \ell_{1}^{\prime} \prime_{2}^{\prime}}^{L}$. After substitution of the expressions given in Eqs. (20), (21) and (26), it is found that the first and third conditions of Eq. (30) are identically satisfied while the second reduces to the one given in Eq. (28) with the upper sign. This confirms the earlier statement that a given intrinsic shape leads to unique conditions on the single-boson energies and interaction matrix elements, independent of the orientation of that shape in the laboratory frame The result provides an additional and independent check on the correctness of all the equations involved in this comparison. Therefore, the analysis henceforth can be restricted to the cases (i) and (ii) of octahedral and cubic intrinsic shape.

### 4.3 Minima with octahedral symmetry

So far, no constraints are found on the single-boson energies $\epsilon_{\ell}$ and interaction matrix elements $v_{\ell_{1} \ell_{2} \ell_{1}^{\prime} \ell_{2}^{\prime}}^{L}$ since Eq. (28) has always a real, positive solution, either for $\delta_{4}^{*}=0$ or for $\delta_{4}^{*}=\pi$, except in the pathological case of no $s-g$ mixing mentioned in Sect. 4.2. Constraints are found by requiring that the extremum is a minimum or, equivalently, that the eigenvalues of the stability matrix are all non-negative. No conditions follow from second derivatives involving $\gamma_{2}$ and $\gamma_{4}$ at a critical point $o^{*}$ with octahedral symmetry. Furthermore, the second derivatives involving $\beta_{4}$ are decoupled from those pertaining to $\beta_{2}$ and $\delta_{4}$, that is, the following equations are identically satisfied:

$$
\begin{equation*}
\left.\frac{\partial^{2} E}{\partial \beta_{2} \partial \beta_{4}}\right|_{o^{*}}=\left.\frac{\partial^{2} E}{\partial \beta_{4} \partial \delta_{4}}\right|_{o^{*}}=0 \tag{31}
\end{equation*}
$$

so that the stability in $\beta_{4}$ follows from the inequality

$$
\begin{equation*}
\left.\frac{\partial^{2} E}{\partial \beta_{4}^{2}}\right|_{o^{*}} \geq 0 \tag{32}
\end{equation*}
$$

Some insight can be obtained by assuming the odd powers of $\beta_{4}^{*}$ to be zero, $c_{03}^{00}=0$, in which case the condition (32) reduces to

$$
\begin{equation*}
\frac{\left(2 c_{00}^{\prime}-c_{02}^{\prime}\right)\left(c_{00}^{\prime}-c_{02}^{\prime}+c_{04}^{\prime}+19 c_{04}^{00}\right)}{-c_{02}^{\prime}+2 c_{04}^{\prime}+38 c_{04}^{00}} \geq 0 . \tag{33}
\end{equation*}
$$

Since the combinations $2 c_{00}^{\prime}-c_{02}^{\prime}$ and $-c_{02}^{\prime}+2 c_{04}^{\prime}+38 c_{04}^{00}$ must have the same sign (see Sect. 4.2), it follows that the conditions

$$
\begin{equation*}
2 c_{00}^{\prime}-c_{02}^{\prime} \geq 0, \quad-c_{02}^{\prime}+2 c_{04}^{\prime}+38 c_{04}^{00} \geq 0 \tag{34}
\end{equation*}
$$

are necessary and sufficient for the energy surface $E\left(\beta_{2}, \beta_{4}, \gamma_{2}, \gamma_{4}, \delta_{4}\right)$ to have an extremum at non-zero hexadecapole deformation which is stable in $\beta_{4}$.

The stability in $\beta_{2}$ and $\delta_{4}$ follows from the diagonal derivatives,

$$
\begin{align*}
\left.\frac{\partial^{2} E}{\partial \beta_{2}^{2}}\right|_{o^{*}}= & \frac{-4 c_{00}^{\prime}+2 c_{20}^{\prime} \pm 2 c_{21}^{00} \beta_{4}^{*}-\left(4 c_{02}^{\prime}-2 c_{20}^{\prime}-2 c_{22}^{\prime}\right) \beta_{4}^{* 2}}{} \\
& \frac{\mp\left(28 c_{03}^{00}-2 c_{21}^{00}\right) \beta_{4}^{* 3}-\left(4 c_{04}^{\prime}-2 c_{22}^{\prime}+76 c_{04}^{00}\right) \beta_{4}^{* 4}}{\left(1+\beta_{4}^{* 2}\right)^{3}}, \\
\left.\frac{\partial^{2} E}{\partial \delta_{4}^{2}}\right|_{o^{*}}= & \frac{\mp 15 c_{03}^{00} \beta_{4}^{* 3}-280 c_{04}^{00} \beta_{4}^{* 4}}{\left(1+\beta_{4}^{* 2}\right)^{2}} . \tag{35}
\end{align*}
$$

These equations are coupled, however, since the off-diagonal derivative generally is non-zero,

$$
\begin{equation*}
\left.\frac{\partial^{2} E}{\partial \beta_{2} \partial \delta_{4}}\right|_{o^{*}}=\frac{2 c_{12}^{1-1} \beta_{4}^{* 2} \pm 7 c_{13}^{1-1} \beta_{4}^{* 3}}{\left(1+\beta_{4}^{* 2}\right)^{2}} . \tag{36}
\end{equation*}
$$

Again, simplifications arise if the coefficients of the odd powers of $\beta_{4}^{*}$ vanish, $c_{03}^{00}=c_{21}^{00}=0$. If, in addition, the off-diagonal derivative vanishes, $c_{12}^{1-1}=$ $c_{13}^{1-1}=0$, the stability in $\beta_{2}$ and $\delta_{4}$ at the hexadecapole deformation $\beta_{4}^{*}$ given by Eq. (29) is guaranteed by the following conditions:

$$
\begin{equation*}
\left(c_{02}^{\prime}-c_{20}^{\prime}\right)\left(-c_{02}^{\prime}+c_{22}^{\prime}\right)+\left(2 c_{00}^{\prime}-c_{20}^{\prime}\right)\left(2 c_{04}^{\prime}-c_{22}^{\prime}+38 c_{04}^{00}\right) \leq 0, \tag{37}
\end{equation*}
$$

and

$$
\begin{equation*}
c_{04}^{00} \leq 0, \tag{38}
\end{equation*}
$$

respectively, where use has been made of the conditions (34), required to have an extremum which is stable in $\beta_{4}$.

Provided that $c_{03}^{00}=c_{21}^{00}=c_{12}^{1-1}=c_{13}^{1-1}=0$, Eqs. (34), (37) and (38) are the necessary and sufficient conditions for the energy surface $E\left(\beta_{2}, \beta_{4}, \gamma_{2}, \gamma_{4}, \delta_{4}\right)$ to have a local minimum with octahedral symmetry. It is not necessarily a unique minimum and it may not be the global one. In particular, the conditions do not exclude the existence of a quadrupole-deformed minimum with $\beta_{2} \neq 0$ at some hexadecapole deformation which differs from $\beta_{4}^{*}$ given in Eq. (29). To exclude the latter possibility for all $\beta_{4}^{*}$, the following stronger conditions must hold [see the first of Eqs. (35)]:

$$
\begin{equation*}
2 c_{00}^{\prime}-c_{20}^{\prime} \leq 0, \quad 2 c_{02}^{\prime}-c_{20}^{\prime}-c_{22}^{\prime} \leq 0, \quad 2 c_{04}^{\prime}-c_{22}^{\prime}+38 c_{04}^{00} \leq 0, \tag{39}
\end{equation*}
$$



Fig. 2. Illustration of the energy surface $E\left(\beta_{2}, \beta_{4}, \gamma_{2}, \gamma_{4}, \delta_{4}\right)$ of Eq. (25) with coefficients $c_{00}^{\prime}=-0.2, c_{20}^{\prime}=-0.5, c_{02}^{\prime}=-1, c_{40}^{\prime}=0, c_{22}^{\prime}=-0.25, c_{04}^{\prime}=0.15$ and $c_{04}^{00}=-0.02$, in arbitrary energy units times $N(N-1)$. Left: $\left(\beta_{2}, \beta_{4}\right)$ plot for $\gamma_{2}=\gamma_{4}=\delta_{4}=0$. Right: $\left(\beta_{4}, \delta_{4}\right)$ plot for $\beta_{2}=0$ and $\gamma_{2}=\gamma_{4}=0$. Blue areas correspond to low energies.
still assuming that $c_{03}^{00}=c_{21}^{00}=0$. These stronger conditions can be combined with the inequalities (34) to yield, with the help of Eq. (26),

$$
\begin{equation*}
c_{02}+\epsilon_{g}^{\prime \prime} \leq 2 c_{00} \leq c_{20}+\epsilon_{d}^{\prime \prime}, \quad c_{02} \leq 2 c_{04}+38 c_{04}^{00}+\epsilon_{g}^{\prime \prime} \leq c_{22}+\epsilon_{d}^{\prime \prime} \tag{40}
\end{equation*}
$$

where $\epsilon_{\ell}^{\prime \prime}$ are the scaled single-boson energies relative to the $s$ boson, $\epsilon_{\ell}^{\prime \prime} \equiv$ $\epsilon_{\ell}^{\prime}-\epsilon_{s}^{\prime}$. These conditions have the advantage to be sufficiently simple to allow an intuitive understanding. With reference to Eqs. (20) and (21), the inequalities (40) express the condition that (i) the $s-g$ mixing is strong enough as compared to the energy difference $\epsilon_{g}-\epsilon_{s}$ to develop a hexadecapole deformed minimum and (ii) the $s-d$ and $d-g$ mixing is sufficiently weak as compared to the energy differences $\epsilon_{s}-\epsilon_{d}$ and $\epsilon_{g}-\epsilon_{d}$, respectively, so as the minimum to remain at $\beta_{2}=0$.

In Fig. 2 an example is shown of an energy surface $E\left(\beta_{2}, \beta_{4}, \gamma_{2}, \gamma_{4}, \delta_{4}\right)$ with coefficients in Eq. (25) that satisfy the conditions (34), (37) and (38). It is obviously not possible to display a five-dimensional surface in its full complexity and judiciously chosen two-dimensional intersections must be shown to illustrate the structure of $E\left(\beta_{2}, \beta_{4}, \gamma_{2}, \gamma_{4}, \delta_{4}\right)$. In the study of shapes with octahedral symmetry one may take $\gamma_{2}=\gamma_{4}=0$ since there is no dependence on these variables at the minimum. Figure 2 shows two intersections, in the $\left(\beta_{2}, \beta_{4}\right)$ plane with $\delta_{4}=0$ and in the ( $\beta_{4}, \delta_{4}$ ) plane with $\beta_{2}=0$, and confirms the existence of two minima with octahedral symmetry for $\beta_{2}^{*}=0$ and $\beta_{4}^{*} \neq 0$, with $\delta_{4}^{*}=0$ and $\delta_{4}^{*}=\pi$, corresponding to an octahedron and a cube, respectively. A third minimum is seen at $\delta_{4}^{*}=\pi / 2$ which represents a shape with a lower discrete symmetry.

## 5 Conclusions

In this paper a general Hamiltonian of the $s d g$-IBM with up to two-body interactions was analyzed as regards the question of the occurrence of intrinsic shapes with octahedral symmetry. Such an analysis requires the use of the most general $s d g$ coherent state (16), leading to a classical energy surface of the generic form (25). A stability analysis of this surface leads to a set of conditions, Eqs. (34), (37) and (38), which are necessary and sufficient for the occurrence of a minimum with an intrinsic shape with octahedral symmetry.

Due to the complicated nature of the stability conditions, only qualitative conclusions have been drawn at this point with regard to the occurrence of octahedral shapes in the $s d g$-IBM. More concrete conclusions will be drawn in the study of a simpler $s d g$-Hamiltonian, which has the advantage of exhibiting dynamical symmetries and which is the topic of another paper in this series.

## Acknowledgements

This work has been carried out in the framework of a CNRS/DEF agreement, project N 13760 .

## References

[1] A. Bohr, B.R. Mottelson, Nuclear Structure. II Nuclear Deformations, Benjamin, New York, 1975.
[2] L.P. Gaffney et al., Nature 497 (2013) 199.
[3] M. Hamermesh, Group Theory and Its Application to Physical Problems, Addison-Wesley, Reading, Massachusetts, 1964.
[4] X. Li, J. Dudek, Phys. Rev. C 49 (1994) 1250(R).
[5] J. Dudek, A. Góźdź, N. Schunck, M. Miśkiewicz, Phys. Rev. Lett. 88 (2002) 252502.
[6] J. Dudek, A. Góźdź, N. Schunck, Acta Phys. Pol. B 34 (2003) 2491.
[7] J. Dudek, D. Curien, N. Dubray, J. Dobaczewski, V. Pangon, P. Olbratowski, N. Schunck, Phys. Rev. Lett. 97 (2006) 072501.
[8] D. Rouvel, Essai sur les Symétries Géométriques et les Transitions de Forme du Noyau de l'Atome, PhD thesis, University of Strasbourg, 2014, unpublished.
[9] A. Bohr, B.R. Mottelson, Nuclear Structure. I Single-Particle Motion, Benjamin, New York, 1969.
[10] L. Landau, E. Lifchitz, Physique Théorique. III Mécanique Quantique, Editions MIR, Moscow, 1967.
[11] S. Takami, K. Yabana, M. Matsuo, Phys. Lett. B 431 (1998) 242.
[12] M. Yamagami, K. Matsuyanagi, M. Matsuo, Nucl. Phys. A 693 (2001) 579.
[13] N. Schunck, J. Dudek, A. Góźdź, P.H. Regan, Phys. Rev. C 69 (2004) 061305(R).
[14] D. Curien, J. Dudek, K. Mazurek, J. Phys.: Conf. Ser. 205 (2010) 012034.
[15] D. Curien, Recherche Expérimentale des Symétries de Haut-Rang en Structure Nucléaire, Habilitation à Diriger des Recherches, University of Strasbourg, 2011, unpublished.
[16] M. Jentschel, W. Urban, J. Krempel, D. Tonev, J. Dudek, D. Curien, B. Lauss, G. de Angelis, P. Petkov, Phys. Rev. Lett. 104 (2010) 222502.
[17] D.M. Brink, Proc. Int. School of Physics, Enrico Fermi Course XXXVI, Varenna, ed. C. Bloch (Academic Press, New York, 1966) p. 247.
[18] R. Bijker, F. Iachello, Phys. Rev. C 61 (2000) 067305.
[19] R. Bijker, F. Iachello, Ann. Phys. (NY) 298 (2002) 334.
[20] R. Bijker, F. Iachello, Phys. Rev. Lett. 112 (2014) 152501.
[21] D.J. Marín-Lámbarri, R. Bijker, M. Freer, M. Gai, Tz. Kokalova, D.J. Parker, C. Wheldon, Phys. Rev. Lett. 113 (2014) 012502.
[22] A. Arima, F. Iachello, Phys. Rev. Lett. 35 (1975) 1069.
[23] F. Iachello, A. Arima, The Interacting Boson Model, Cambridge University Press, Cambridge, 1987.
[24] A. Arima, F. Iachello, Ann. Phys. (NY) 99 (1976) 253.
[25] A. Arima, F. Iachello, Ann. Phys. (NY) 111 (1978) 201.
[26] O. Scholten, F. Iachello, A. Arima, Ann. Phys. (NY) 115 (1978) 325.
[27] J. Engel, F. Iachello, Phys. Rev. Lett. 54 (1985) 1126.
[28] W. Nazarewicz, P. Rozmej, Nucl. Phys. A 369 (1981) 396.
[29] S.G. Rohoziński, A. Sobiczewski, Acta Phys. Pol. B 12 (1981) 1001.
[30] J. Dudek, A. Góźdź, K. Mazurek, H. Molique, J. Phys. G 37 (2010) 064032.
[31] Y.D. Devi, V.K.B. Kota, Pramana J. Phys. 39 (1992) 413.
[32] R. Gilmore, J. Math. Phys. 20 (1979) 891.
[33] J.N. Ginocchio, M.W. Kirson, Phys. Rev. Lett. 44 (1980) 1744.
[34] A.E.L. Dieperink, O. Scholten, F. Iachello, Phys. Rev. Lett. 44 (1980) 1747.
[35] Y.D. Devi, V.K.B. Kota, Z. Phys. A 337 (1990) 15.
[36] J.N. Ginocchio, M.W. Kirson, Nucl. Phys. A 350 (1980) 31.
[37] P. Van Isacker, A. Bouldjedri, S. Zerguine, Nucl. Phys. A 836 (2010) 224.
[38] P. Van Isacker, J.-Q. Chen, Phys. Rev. C 24 (1981) 684.

