Intrinsic structure of two-phonon states in the interacting boson model

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Abstract

A general study of excitations up to two-phonon states is carried out using the intrinsic-state formalism of the Interacting Boson Model (IBM). Spectra and transitions for the different dynamical symmetries are analyzed and the correspondence with states in the laboratory frame is established. The influence of multi-phonon states is discussed. The approach is useful in problems where the complexity of the IBM spectrum renders the analysis in the laboratory frame difficult.
I. INTRODUCTION

Whether double-$\gamma$ excitations exist or not in nuclei has been under discussion during the last 30 years. Double-$\gamma$ excitations correspond to $K^\pi = 0^+$ and $K^\pi = 4^+$ states, and are the bandheads of two rotational bands superimposed on the vibrational spectrum. Recent experimental improvements in nuclear spectroscopy following Coulomb excitation [1], inelastic neutron scattering [2] and thermal-neutron capture [3] have made possible the study of highly excited low-spin states which until now had been inaccessible. In transitional even–even nuclei $^{186-192}$Os and $^{194}$Pt large components of the double-$\gamma$ excitation have been identified [4,5]. In well-deformed nuclei the search for double-$\gamma$ excitations has led to the identification of a first candidate namely the $K^\pi = 4^+$ level at 2055 keV in $^{168}$Er [3]. Subsequently, other two-phonon excitations have been observed. For example, based on their decay properties the levels in $^{166}$Er at excitation energies of 1943 and 2028 keV were judged to be collective and interpreted as $K^\pi = 0^+$ and $K^\pi = 4^+$ members of the double-$\gamma$ multiplet, respectively [7,8]. Other examples of double-$\gamma$ excitations are the $K^\pi = 4^+$ state at 1435 keV in $^{106}$Mo [4], $K^\pi = 4^+$ states in $^{154-156}$Gd [10] or $K^\pi = 4^+$ state at 2173 keV in $^{164}$Dy [11]. It should be noted, however, that the identification of such states as members of a two-phonon multiplet is still very much under debate [12].

A possible framework for investigating two-phonon excitations is the Interacting Boson Model (IBM) [13]. This model has been very successful in describing low-lying collective spectra in medium-mass and heavy nuclei. Two-phonon excitations are present in the IBM but the analysis of their properties is not so easy to carry out in the laboratory frame since in the energy region of interest (around 2 MeV) the density of states is high and their decay properties are intricate. For example, it is as yet not clear how and, if so, to what extent anharmonicities can be introduced in the model, a question that did generate controversy in the early days of the model [14,15].

In this paper it is shown that the intrinsic-state formalism [16,17] provides an ideal framework for analysing the problem of two-phonon excitations in the IBM. The intrinsic-state
formalism is an approximation (of order 1/N) to the exact IBM, but its advantage is that it gives a clear interpretation of the structure of the states. In order to address the problem of two-phonon excitations we present here calculations in the Tamm–Dancoff Approximation (TDA), extended up to two-particle–two-hole excitations carried in the intrinsic frame of the IBM. This approximation is useful due to its simplicity and its physical transparency, and it allows to derive analytical expressions for energies and electromagnetic transitions applicable to a wide range of situations.

The structure of the paper is as follows. First, a brief recapitulation of the intrinsic-state formalism as applied to the IBM is given, which is subsequently extended to include up to two-phonon excitations. Problems related to spurious states and anharmonicity are discussed. In section II the results of schematic calculations in the intrinsic frame are compared with those in the laboratory frame for the three dynamical symmetry limits of the IBM. The character of the two-phonon states is established. Section IV is devoted to electromagnetic transitions. Finally, in section V conclusions of this work are presented.

II. THE IBM IN THE INTRINSIC FRAME

The IBM describes low-lying collective excitations in even–even nuclei in terms of bosons with angular momentum 0 (s bosons) and 2 (d bosons). These bosons interact via a hamiltonian that is rotational invariant and number conserving and usually includes up to two-body interactions, although higher-order terms have been sometimes included. The most general two-body IBM hamiltonian may be written in multipole form as

$$H = \varepsilon_s \hat{n}_s + \varepsilon_d \hat{n}_d + \kappa_0 \hat{P}^\dagger \hat{P} + \sum_{L=1}^{4} \kappa_L \hat{T}_L \cdot \hat{T}_L,$$

(1)

where

$$P^\dagger = \frac{1}{2} d^\dagger \cdot d^\dagger - \frac{1}{2} s^\dagger \cdot s^\dagger$$

(2)

and
\[ T_{LM} = \sum_{\ell_1 \ell_2} \chi^{L}_{\ell_1 \ell_2} (\gamma_{\ell_1}^\dagger \times \gamma_{\ell_2})_{LM}, \]  

\[(3)\]

with \[
\begin{align*}
\chi^{1}_{00} &= 0, \quad \chi^{1}_{02} = 0, \quad \chi^{1}_{20} = 0, \quad \chi^{1}_{22} = 1 \\
\chi^{2}_{00} &= 0, \quad \chi^{2}_{02} = 1, \quad \chi^{2}_{20} = 1, \quad \chi^{2}_{22} = \chi \\
\chi^{3}_{00} &= 0, \quad \chi^{3}_{02} = 0, \quad \chi^{3}_{20} = 0, \quad \chi^{3}_{22} = 1 \\
\chi^{4}_{00} &= 0, \quad \chi^{4}_{02} = 0, \quad \chi^{4}_{20} = 0, \quad \chi^{4}_{22} = 1
\end{align*}\]

\[(4)\]

The symbol \( \cdot \) denotes scalar product, in this work the scalar product is defined as \( \hat{T}_L \cdot \hat{T}_L = \sum_{M} (-1)^{L-M} \hat{T}_{LM} \hat{T}_{L-M} \), while \( \gamma \) with \( \ell = 0 (\ell = 2) \) corresponds to an s boson (d boson). In Eq. (3) the operator \( \gamma_{\ell m} = (-1)^{\ell-m} \gamma_{\ell-m} \) is introduced so as to verify the appropriate properties with respect to spatial rotations.

The intrinsic-state formalism \[16,17\] provides a connection between the IBM and the Bohr–Mottelson collective model \[18\]. Let us consider a system consisting of a large but finite number \( N \) of interacting bosons. The dynamical behaviour of this system can be described in lowest-order as arising from independent bosons moving in an average field. In this approximation, the ground state of such a system is a condensate \( |c\rangle \) of bosons, all occupying a single state \( \Gamma^c_\ell \) of lowest energy,

\[ |c\rangle = \frac{1}{\sqrt{N!}} (\Gamma^c_\ell)^N |0\rangle, \]  

\[(5)\]

where \[
\Gamma^c_\ell = \frac{1}{\sqrt{1 + \beta^2}} \left( s^\dagger + \beta \cos \gamma d^\dagger_0 + \frac{1}{\sqrt{2}} \beta \sin \gamma (d^\dagger_2 + d^\dagger_{-2}) \right). \]  

\[(6)\]

The dynamical variables \( \beta \) and \( \gamma \) are related to the quadrupole shape variables of the geometrical model \[18\] (\( \beta \geq 0 \)). The expectation value of the IBM hamiltonian \[1\] in the ground state (5) is

\[ \langle c | H | c \rangle = \frac{N}{5(1 + \beta^2)} \left( 5 \varepsilon_s + 25 \kappa_2 + \beta^2 (5 \varepsilon_d - 3 \kappa_1 + 5 \kappa_2 + 5 \chi^2 \kappa_2 - 7 \kappa_3 + 9 \kappa_4) \right) \]

\[+ \frac{N(N - 1)}{140(1 + \beta^2)^2} \left( 35 \kappa_0 + \beta^2 (-70 \kappa_0 + 560 \kappa_2) - 80 \sqrt{14} \beta^3 \chi \cos(3 \gamma) \kappa_2 
+ \beta^4 (35 \kappa_0 + 40 \chi^2 \kappa_2 + 72 \kappa_4) \right). \]  

\[(7)\]
Alternative expressions can be found in Refs. [16,19,20] using normal-ordered hamiltonians. The equilibrium values of the deformation parameters are obtained by minimizing the energy expression (7) with respect to $\beta$ and $\gamma$. Due to physical considerations a minimum for $\beta \to \infty$ must be excluded [20]. Furthermore it follows from (7) that a triaxial minimum is excluded and only prolate ($\gamma = 0^\circ$) or oblate ($\gamma = 60^\circ$) solutions are allowed. For an attractive quadrupole force ($\kappa_2 < 0$) these are found for $\chi < 0$ and $\chi > 0$, respectively. A special situation of $\gamma$-unstability occurs if the quadrupole term vanishes ($\kappa_2 = 0$) or if $\chi = 0$.

The condensed boson $\Gamma_p^\dagger$ (8) is the first component of a new boson basis (deformed or intrinsic bosons). These deformed bosons are related to the spherical ones (laboratory bosons) through a general unitary transformation $\eta$,

$$
\Gamma_p^\dagger = \sum_{\ell m} \eta^p_{\ell m} \gamma^\dagger_{\ell m}, \qquad \gamma^\dagger_{\ell m} = \sum_p \eta^p_{\ell m} \Gamma_p^\dagger,
$$

the deformation parameters $\eta^p_{\ell m}$ verifying the orthonormalization conditions

$$
\sum_{\ell m} \eta^{p*}_{\ell m} \eta^p_{\ell m} = \delta_{pp'}, \quad \sum_p \eta^{p*}_{\ell m} \eta^{p'}_{\ell m'} = \delta_{\ell\ell'} \delta_{mm'}.
$$

The index $p$ labels the different deformed bosons. After obtaining the $\eta$ parameters for $p = c$ (i.e. the equilibrium deformation parameters), the $\eta$ parameters for the excited bosons follow from the orthogonality conditions (4). An appropriate choice of deformed bosons can be found in Ref. [20]:

$$
\begin{align*}
\eta_{00}^c &= \frac{1}{\sqrt{1 + \beta^2}} , & \eta_{20}^c &= \frac{\beta \cos \gamma}{\sqrt{1 + \beta^2}} , & \eta_{22}^c &= \eta_{2-2}^c = \frac{\beta \sin \gamma}{\sqrt{2\sqrt{1 + \beta^2} \sin \gamma}}, \\
\eta_{00}^\beta &= \frac{-\beta}{\sqrt{1 + \beta^2}} , & \eta_{20}^\beta &= \frac{\cos \gamma}{\sqrt{1 + \beta^2}} , & \eta_{22}^\beta &= \eta_{2-2}^\beta = \frac{\sin \gamma}{\sqrt{2\sqrt{1 + \beta^2}}}, \\
\eta_{20}^{\gamma+} &= -\sin \gamma , & \eta_{22}^{\gamma+} &= \eta_{2-2}^{\gamma+} = \frac{\cos \gamma}{\sqrt{2}}, \\
\eta_{21}^c &= \frac{1}{\sqrt{2}} , & \eta_{2-1}^c &= \frac{1}{\sqrt{2}} , \\
\eta_{21}^\gamma &= \frac{1}{\sqrt{2}} , & \eta_{2-1}^\gamma &= -\frac{1}{\sqrt{2}}, \\
\eta_{22}^{\gamma-} &= \frac{1}{\sqrt{2}} , & \eta_{2-2}^{\gamma-} &= -\frac{1}{\sqrt{2}},
\end{align*}
$$

other coefficients being zero. This basis has a clear correspondence with the usual $\beta$ and $\gamma$ excitations.
In the following section the usefulness of this notation for the calculation of matrix elements in a one- and two-phonon basis shall become clear.

A. One- and two-phonon states

The excited bands can be considered as intrinsic excitations built on the boson condensate (3), obtained by replacing a $c$ boson by an excited one, two $c$ bosons by two excited ones and so on. This set of excitations contains spurious states that are coupled to the true physical ones and must be removed [20]. This problem is a consequence of TDA. In the Random Phase Approximation (RPA) all the spurious states come out with zero energy and are decoupled from the physical states [21]. However, RPA is more difficult to implement than TDA and obscures any physical interpretation. The problem of the spurious states will be returned to later.

The excited states included in the present analysis are

$$|p\rangle = \frac{1}{\sqrt{(N-1)!}} \Gamma_p^\dagger (\Gamma^\dagger c)^{N-1} |0\rangle,$$

$$|p\ p'\rangle = \frac{1}{\sqrt{1 + \delta_{p,p'}}} \frac{1}{\sqrt{(N-2)!}} \Gamma_p^\dagger \Gamma_{p'}^\dagger (\Gamma^\dagger c)^{N-2} |0\rangle,$$$$
\tag{11}$$

where $p, p' \neq c$. Eigenfunctions are linear combinations of these excited states plus the ground state,

$$|\phi^\xi\rangle = N^\xi \left( W^\xi |c\rangle + \sum_p X^\xi_p |p\rangle + \sum_{pp'} Y^\xi_{pp'} |pp'\rangle \right),$$

$$\tag{12}$$

where $N^\xi$ is a normalization constant. The ground-state contribution comes from the off-diagonal matrix elements of the Hamiltonian between the ground state and the two-phonon states.

To obtain the states (12), the Hamiltonian is diagonalized in the basis of excited states (11) plus the ground state (3). The different matrix elements that intervene are

$$\langle c | H | p \rangle = \sqrt{N} F_{cp}^{(1)} + 2 \sqrt{N} (N - 1) F_{cpp}^{(2)} = 0,$$

$$\tag{13}$$
The coefficients \( \tilde{\varepsilon} \) where

\[
\langle c|H|pp' \rangle = \frac{2\sqrt{N} \sqrt{N-1}}{\sqrt{1 + \delta_{pp'}}} F_{cpp'}^{(2)}, \tag{14}
\]

\[
\langle p|H|p' \rangle = F_{pp'}^{(1)} + 4(N - 1) F_{cpp'}^{(2)} + \delta_{pp'}(N - 1) \left( F_{cc}^{(1)} + (N - 2) F_{cccc}^{(2)} \right), \tag{15}
\]

\[
\langle p|H|p''p''' \rangle = \frac{\sqrt{N - 1}}{\sqrt{1 + \delta_{p''p'''}}} \left( 4 F_{cpp'p''}^{(2)} + \delta_{pp'} F_{cp'}^{(1)} + \delta_{pp''} F_{cpp'}^{(1)} \right.
\]
\[
+ 2(N - 2) \left( \delta_{pp'} F_{cpp''}^{(2)} + \delta_{pp''} F_{cpp'}^{(2)} \right) \bigg); \tag{16}
\]

\[
\langle pp'|H|p''p''' \rangle = \frac{\delta_{pp''} \delta_{p''p'''} + \delta_{pp'''} \delta_{p''p'''}}{1 + \delta_{pp'} \delta_{pp''} \delta_{p''p'''} \left( (N - 2) F_{cc}^{(1)} + (N - 2)(N - 3) F_{cccc}^{(2)} \right)}
\]
\[
+ \frac{1}{\sqrt{(1 + \delta_{pp'})(1 + \delta_{p''p'''})}} \left\{ 4 F_{pp'p''p'''p'''}^{(2)} + \delta_{pp''} \left( F_{p'p''p''}^{(1)} + 4(N - 2) F_{cpp'''}^{(2)} \right) \right.
\]
\[
+ \delta_{pp'''} \left( F_{pp'p'''}^{(1)} + 4(N - 2) F_{cpp''}^{(2)} \right) + \delta_{p''p'''} \left( F_{pp''p'''}^{(1)} + 4(N - 2) F_{cpp''}^{(2)} \right) \left\} ; \tag{17}
\]

where

\[
F_{pp'}^{(1)} = \sum_{\ell_1 m_1} \tilde{\varepsilon}_{\ell_1} \eta_{\ell_1 m_1}^{pp} \eta'_{\ell_1 m_1} \tag{18}
\]

and

\[
F_{p_1 p_2 p_3 p_4}^{(2)} = \sum_{\ell_1 m_1 \ell_2 m_2 \ell_3 m_3 \ell_4 m_4} V_{\ell_1 m_1, \ell_2 m_2, \ell_3 m_3, \ell_4 m_4} \eta_{p_1}^{\ell_1 m_1} \eta_{p_2}^{\ell_2 m_2} \eta_{p_3}^{\ell_3 m_3} \eta_{p_4}^{\ell_4 m_4}. \tag{19}
\]

The coefficients \( \tilde{\varepsilon}_\ell \) include the single-particle energies \( \varepsilon_\ell \) plus contributions from the two-body terms in the IBM hamiltonian \([1]\). The coefficients \( V_{\ell_1 m_1, \ell_2 m_2, \ell_3 m_3, \ell_4 m_4} \) are defined as

\[
V_{\ell_1 m_1, \ell_2 m_2, \ell_3 m_3, \ell_4 m_4} \equiv \frac{1}{4} \langle \ell_1 m_1, \ell_2 m_2 | V | \ell_3 m_3, \ell_4 m_4 \rangle \sqrt{1 + \delta_{\ell_1 \ell_2} \delta_{m_1 m_2} \sqrt{1 + \delta_{\ell_1 \ell_4} \delta_{m_3 m_4}}} . \tag{20}
\]

By construction \( F_{pp'}^{(1)} \) is symmetric under interchange of \( p \) and \( p' \) and \( F_{p_1 p_2 p_3 p_4}^{(2)} \) has the same symmetry properties as \( V_{\ell_1 m_1, \ell_2 m_2, \ell_3 m_3, \ell_4 m_4} \).
B. Spurious modes. Goldstone bosons

Before diagonalization spurious bosons must be removed from the basis. The procedure to separate out those modes from the physical ones is described in detail in Ref. [20]. In this section we just enumerate the spurious (Goldstone) modes that occur in the different geometrical limits of the IBM.

- $\beta = 0$, spherical nuclei.
  - $O(3)$ or $O(5)$ scalar hamiltonian. There are no Goldstone bosons.
  - $O(6)$ scalar hamiltonian. A spherical nucleus corresponds to the $U(5)$ dynamical symmetry, not compatible with a symmetry group $O(6)$. Therefore this possibility must be excluded.

- $\beta > 0$, deformed nuclei.
  - $O(3)$ scalar hamiltonian. For $\gamma = 0$, $\Gamma_x$ and $\Gamma_y$ are spurious bosons. For $\gamma = \pi/3$ the spurious bosons are $\Gamma_x$ and $\Gamma_{\gamma-}$. In the triaxial case $\Gamma_x$, $\Gamma_y$ and $\Gamma_{\gamma-}$ are Goldstone bosons.
  - $O(5)$ scalar hamiltonian. All the excited bosons are spurious except the $\Gamma_\beta$ boson.
  - $O(6)$ scalar hamiltonian. All the excited bosons correspond to Goldstone bosons.

C. The anharmonicity problem

It is not clear a priori to what extent $\beta$ and $\gamma$ vibrations are harmonic in the IBM. The analysis of this problem is quite difficult in the laboratory frame; with the intrinsic-state formalism, however, some general conclusions can be obtained for arbitrary hamiltonians.

Let us consider a system with a large number of bosons $N$. For large $N$ the IBM hamiltonian is approximately diagonal in the basis of excited states $|\Gamma\rangle$. The degree of anharmonicity $\varsigma$ can be defined as (with this definition the harmonic limit corresponds to $\varsigma = 0$)
ς = \frac{E_{p}^{ex} \, E_{p}^{ex}}{E_{p}^{ex}} - 2, \quad (21)

with

E_{p}^{ex} = \langle p|H|p \rangle - \langle c|H|c \rangle, \quad (22)

E_{p}^{ex} = \langle pp|H|pp \rangle - \langle c|H|c \rangle. \quad (23)

These can be evaluated with the help of the following expressions, in which a Hamiltonian including up to three-body interactions have been supposed,

\langle c|H|c \rangle = N(N-1)(N-2)F^{(3)}_{cccccc} + N(N-1)F^{(2)}_{cccc} + NF^{(1)}_{cc}, \quad (24)

\langle p|H|p \rangle = (N-1)(N-2)(N-3)F^{(3)}_{cccccc} + (N-1)(N-2)F^{(2)}_{cccc} + 9(N-2)(N-3)F^{(3)}_{ccppcc}

+ (N-1) \left( F^{(1)}_{cc} + 4F^{(2)}_{pccp} \right) + F^{(1)}_{pp}, \quad (25)

\langle pp|H|pp \rangle = (N-2)(N-3)(N-4)F^{(3)}_{cccccc} + (N-2)(N-3) \left( F^{(2)}_{cccc} + 18F^{(3)}_{ccppppc} \right)

+ (N-2) \left( F^{(1)}_{cc} + 8F^{(2)}_{pccp} + 18F^{(3)}_{cppppc} \right) + 2F^{(1)}_{pp} + 2F^{(2)}_{pppp}, \quad (26)

where \( F^{(1)} \) and \( F^{(2)} \) are defined in Eqs. (18) and (19), and \( F^{(3)} \) equals

\begin{equation}
F^{(3)}_{p_{1}p_{2}p_{3}p_{4}p_{5}p_{6}} = \sum_{\ell',s,m'} U_{\ell_{1}m_{1},\ell_{2}m_{2},\ell_{3}m_{3},\ell_{4}m_{4},\ell_{5}m_{5},\ell_{6}m_{6}} \eta_{\ell_{1}m_{1}}^{p_{1}} \eta_{\ell_{2}m_{2}}^{p_{2}} \eta_{\ell_{3}m_{3}}^{p_{3}} \eta_{\ell_{4}m_{4}}^{p_{4}} \eta_{\ell_{5}m_{5}}^{p_{5}} \eta_{\ell_{6}m_{6}}, \quad (27)
\end{equation}

where \( U_{\ell_{1}m_{1},\ell_{2}m_{2},\ell_{3}m_{3},\ell_{4}m_{4},\ell_{5}m_{5},\ell_{6}m_{6}} \) are the interaction matrix elements between symmetrized, normalized three-boson states.

With the expressions (21–26) it can be shown that the leading order of \( \varsigma \) is \( 1/N \). Furthermore, this result remains valid for a general IBM Hamiltonian with up to \( n \)-body interactions. The conclusion is thus that anharmonicities can only exist in the IBM for a finite number of bosons. Only in the U(5) limit [22], when some of the coefficients (24–26) exactly vanish, the spectrum can be anharmonic even for infinite \( N \). The harmonicity of the IBM spectra in the limit \( N \to \infty \) will be used as a guide to identify the number of excited bosons in a given state.
III. SCHEMATIC CALCULATIONS

A. Dynamic symmetries

The analysis of the three dynamical symmetry limits of the IBM provides a good test of the formalism presented in the previous section.

In calculations carried out in the laboratory frame it is, in some cases, difficult to identify the character of a band \((\beta, \gamma, \ldots)\). This becomes increasingly difficult as the number of phonons increases. In the intrinsic-frame calculations, on the other hand, the character of the band is easily identified from the structure of the state. For high \(N\) the intrinsic-state formalism provides a good approximation to the exact calculation and it can thus be used to clearly identify the character of the bands in the laboratory frame. For low \(N\) the character of the bands in the laboratory frame can be obtained extrapolating the results of high \(N\).

In the following the intrinsic-state results for the three dynamical symmetry limits of IBM are presented.

• \(U(5)\) limit. The hamiltonian in this limit is

\[
H = \varepsilon_d \hat{n}_d + \sum_{L=1,3,4} \kappa_L \hat{T}_L \cdot \hat{T}_L.
\]  

\[
(28)
\]

It corresponds to the spherical limit \((\beta = 0)\). There are no Goldstone bosons. The ground state is a condensate of \(s\) bosons \((s^\dagger)^N|0\rangle\) and coincides with the exact (laboratory) ground state. Excited bosons correspond to \(d^\dagger\); therefore excited states are equal in the intrinsic and laboratory frames. A calculation in the intrinsic frame thus coincides with the exact one.

• \(SU(3)\) limit. This dynamical symmetry corresponds to the hamiltonian

\[
H = \sum_{L=1,2} \kappa_L \hat{T}_L \cdot \hat{T}_L.
\]  

\[(29)\]

with \(\chi = \pm \sqrt{7}/2\). For prolate nuclei \(\Gamma_x\) and \(\Gamma_y\) are the only Goldstone bosons while, for oblate nuclei, these are \(\Gamma_x\) and \(\Gamma_{\gamma-}\). The analysis of the character of the bands is
especially relevant in this case because the concepts of $\gamma$ and $\beta$ bands are appropriate for this limit or situations close to it, i.e. well-deformed nuclei.

The character of the bands built on one- and two-phonon excitations traditionally has been identified in the laboratory frame in terms of the quantum number $K$ and the most symmetric representations of $SU(3)$ \cite{23}. In this way the $\beta$ band corresponds to the representation $(2N - 4, 2) K = 0$ [where $(\lambda, \mu)$ are the Elliott quantum numbers] and the $\gamma$ band to $(2N - 4, 2) K = 2$. In the case of two-phonon excitations assignments are already less clear. There are four possible two-phonon bands: two with $K = 0$ ($\beta^2$ and $\gamma^2$), one with $K = 2$ ($\beta\gamma$) and one with $K = 4$ ($\gamma^2$). These correspond to the $(2N - 8, 4)$ and the $(2N - 6, 0)$ representations of the $SU(3)$ limit. It is not a priori clear, however, how the bands should be assigned to the $SU(3)$ representations; in particular, this ambiguity exists for the $K = 0$ bands. We now proceed to show how this problem can be solved using the intrinsic-state formalism.

It is worth noting that with the definition of $\gamma^+$ and $\gamma^-$ bosons given in Eq. (10) and the definition of two-phonon states given in Eq. (11), the states with two $\gamma^+$ or two $\gamma^-$ excitations have no good $K$ quantum number for the case of axial symmetry. In order to have good $K$ in that case, a simple linear combination correctly normalized can be done,

\[
|\gamma_{K=0}^2\rangle = \frac{1}{\sqrt{2}} \left[ |\gamma_+^2\rangle + |\gamma_-^2\rangle \right], \tag{30}
\]

\[
|\gamma_{K=4}^2\rangle = \frac{1}{\sqrt{2}} \left[ |\gamma_+^2\rangle - |\gamma_-^2\rangle \right]. \tag{31}
\]

We will work with these states even in the cases in which $K$ is considered not to be a good quantum number.

In Fig. 1 we present a calculation for a particular $SU(3)$ hamiltonian and compare the exact and approximate calculations for a wide range of $N$. In general, to identify the character of an excitation its energy in the intrinsic and laboratory frame should
be compared. This procedure is not unambiguous for low $N$. Therefore, first a large $N$ is considered in which case the excitation energies are proportional to the number of excited phonons, i.e. the spectrum is harmonic (see section II C). For $\kappa_1 = 0$ the eigenenergies of the hamiltonian (29) are

$$E(L, \lambda, \mu) = -\frac{3\kappa_2}{8} L(L+1) + \frac{\kappa_2}{2} (\lambda^2 + \mu^2 + \lambda \mu + 3\lambda + 3\mu).$$

(32)

The $(\lambda, \mu)$ contained in a symmetric representation $[N]$ of $U(6)$ are

$$(\lambda, \mu) = (2N - 4n_x - 6n_y, 2n_x), \quad n_x, n_y = 0, 1, 2, \ldots,$$

(33)

with $2N - 4n_x - 6n_y \geq 0$. Neglecting the $L(L+1)$ term in (32), the excitation energies for the different representations are

$$E(\lambda, \mu) - E(2N, 0) = -\kappa_2(6n_x + 12n_y)N + \kappa_2(6n_x^2 + 18n_y^2 + 18n_xn_y - 3n_x - 9n_y).$$

(34)

From this expression it follows that $\Delta n_x = +1$ corresponds to a single-phonon excitation and $\Delta n_y = +1$ to a double-phonon excitation. So it is clear that the one-phonon excitations are in the $(2N - 4, 2)$ representation while the two-phonon excitations belong to $(2N - 8, 4)$ or $(2N - 6, 0)$.

Finally, to fully determine the character of the states approximate and exact energies are compared and the structure of the state is determined in the intrinsic frame. In this way the mixture between the $\beta^2$ and $\gamma^2_{K=0}$ excitations is found and the result is that $(2N - 8, 4)K = 0$ corresponds to the combination $\sqrt{\frac{2}{3}} \beta^2 + \sqrt{\frac{1}{3}} \gamma^2_{K=0}$ while $(2N - 6, 0)K = 0$ corresponds to $\sqrt{\frac{1}{3}} \beta^2 - \sqrt{\frac{2}{3}} \gamma^2_{K=0}$. If the quadrupole generator of $SU(3)$ is used as E2 operator, no transitions can occur between the two bands because they belong to different $SU(3)$ representations. This result is reproduced in the intrinsic frame since their particular composition prevents E2 transitions between them (see section IV).
• $O(6)$ limit. The Hamiltonian for this limit is

$$H = \kappa_0 \hat{P}^\dagger \hat{P} + \sum_{L=1,3} \kappa_L \hat{T}_L \cdot \hat{T}_L.$$  \hspace{1cm} (35)

A particular case of this Hamiltonian is

$$H = \kappa'_2 \hat{T}_2 \cdot \hat{T}_2,$$  \hspace{1cm} (36)

with $\chi = 0$. This latter form is particularly useful in the study of the transition from $SU(3)$ to $O(6)$ by varying a single parameter $\chi$.

In this limit the concept of $\beta$ and $\gamma$ bands is quite vague and it is therefore difficult to find the bandheads in the spectrum and to identify their character. To determine the number of excited phonons in a given state of the $O(6)$ limit, the harmonicity of the spectrum for high boson number is used (see section II C). States are labeled by $(\sigma, \nu_\Delta, \tau, L)$ \cite{24} and the possible values of $\sigma$ and $\tau$ are,

$$\sigma = N - 2n > 0, \quad n = 0, 1, ..., \quad \tau = \sigma, \sigma - 1, ..., 1, 0.$$  \hspace{1cm} (37)

The eigenenergies in terms of these labels are

$$E(\sigma, \tau, L) = A\sigma(\sigma + 4) + B\tau(\tau + 3) + CL(L + 1),$$  \hspace{1cm} (38)

with for realistic calculations $A < 0$, $B > 0$ and $C > 0$. For these parameters, bandheads correspond to $\tau = 0$ and $L = 0$. Their energy is given by

$$E(\sigma) = A\sigma(\sigma + 4)$$  \hspace{1cm} (39)

and their excitation energy is,

$$E(\sigma = N - 2n) - E(\sigma = N) = 4A(-nN) + 4A(n^2 - 2n).$$  \hspace{1cm} (40)

From the latter expression it follows that $n$ represents the number of excited phonons.
In Fig. 2 a calculation for a particular $O(6)$ Hamiltonian is shown and a comparison of the exact and approximate results for a wide range of $N$ is presented. This limit corresponds to the $\gamma$-unstable vibrator and the only physical excited boson is $\Gamma_\beta$.

**B. Transitional hamiltonians**

In the previous section the degree of accuracy of the method was illustrated. In this section schematic Hamiltonians are analyzed which do not correspond to any of the three dynamical symmetry limits. A fixed number of bosons is used and results are plotted as a function of a parameter in the Hamiltonian that allows to explore a wide range of situations, including presumably unrealistic ones. In these calculations the Goldstone bosons correspond to $\Gamma_x$ and $\Gamma_y$ and have been removed before diagonalization. For some extreme values of the parameters, the ground state contains a sizeable contribution from two-phonon excitations.

Figure 3a shows the results of a calculation with a quadrupole and a pairing interaction ($H = \kappa_0 \hat{P}^\dagger \hat{P} + \kappa_2 \hat{T}_2 \cdot \hat{T}_2$, with $\chi = -\sqrt{7}/2$) for $N = 16$. It is seen that the character of the different bands changes as a function of the ratio $-\kappa_0/\kappa_2$. Note the increase with $-\kappa_0/\kappa_2$ of the energy of the $\beta$ band while the $\gamma$-band energy remains approximately constant and the harmonic behaviour between the one-$\gamma$ and two-$\gamma$ bands holds throughout. This figure displays the same trends as Fig. 14a of Ref. [25] which shows an identical calculation in the laboratory frame. Only small differences occur due to mixing with higher-order phonon excitations. Note that a realistic value of the ratio $-\kappa_0/\kappa_2$ is around 4.

Figure 4a shows the influence of a hexadecapole term added to a quadrupole term ($H = \kappa_2 \hat{T}_2 \cdot \hat{T}_2 + \kappa_4 \hat{T}_4 \cdot \hat{T}_4$, with $\chi = -\sqrt{7}/2$) for $N = 16$. In the whole range of variation of the parameter $\kappa_4/\kappa_2$ there is a clear separation in energy and only small mixing between the one- and two-phonon states. The $SU(3)$ limit is recovered for $\kappa_4 = 0$.

In Fig. 5a a transition from a deformed to a spherical nucleus is analyzed via the Hamiltonian $H = \varepsilon_d \hat{\mu}_d + \kappa_2 \hat{T}_2 \cdot \hat{T}_2$, with $\chi = -\sqrt{7}/2$ for $N = 16$. A sharp transition occurs at a
particular value of the ratio $-\varepsilon_d/\kappa_2$ at which point the equilibrium value of $\beta$ drops from a finite value to zero.

C. Influence of multi-phonon excitations

Besides the mean-field approximation, another approximation made in this study is a truncation in the number of excited phonons that are included in the basis. This number is limited to two here. The previous results indicate that, in the majority of cases, excited states with different phonon number are decoupled. It would be of interest, however, to study the influence of $n$-phonon states with $n > 2$. Some idea of their influence, without actually extending the phonon basis, can be obtained by comparing the previous results (which include $n = 0, 1, 2$) with those where $n = 0, 1$. This is done in Figs. 3, 4 and 5. The conclusion is that the influence of two-phonon on one-phonon states is small except for some extreme parameter values and in regions where the two cross (e.g. for $\kappa_0/\kappa_2 \approx -4$ in Fig. 3).

D. Simulation of triaxiality in mean field theories

In the standard IBM, i.e. with hamiltonians up to two-body operators, a rigid triaxial shape cannot be obtained [16,17,19]. One way to induce triaxiality is to include a cubic term [19] into the hamiltonian. The intrinsic-state formalism supposes the presence of an average field, the characteristics of which should depend self-consistently on the hamiltonian. A simple way to investigate the consequences of triaxiality is to relax the self-consistency requirement and to impose by hand a triaxial mean field through a value $\gamma \neq 0^\circ$. It must be emphasized that in mean-field theories it is allowed to perturb the average field coming from the minimization of the energy.

In Fig. 6 a calculation of this type is illustrated for a simple hamiltonian varying $\gamma$. The value of $\beta$ is obtained minimizing the energy for a fixed $\gamma$. For $\gamma > 15^\circ$ the lowest band loses the character of ground state, i.e. this band is no longer a condensate of $\Gamma_c$ bosons, and the interpretation of the levels becomes more complicated. A intriguing feature of this figure is
that the excitation energies of the two-phonon states are approximately constant whereas the excitation energies of one-phonon states decrease smoothly with $\gamma$. In other words a sizeable anharmonicity occurs for $\gamma \neq 0$. For example, for $\gamma \sim 6^\circ$ the anharmonicity $\varsigma$ (21) is around 0.5. This degree of anharmonicity is observed in $^{166}$Er [18] and $^{168}$Er [14].

This result points towards a link between anharmonicity and triaxiality. For a better understanding of this connection, however, a fully self-consistent calculation should be carried out which includes three-body interactions that induce triaxiality.

**IV. ELECTROMAGNETIC TRANSITIONS**

To calculate electromagnetic transitions in the intrinsic frame one must assume that the total wave function can be separated into intrinsic and rotational (collective) part. This hypothesis is only strictly true for the $SU(3)$ limit but it can be considered as a good approximation in well-deformed nuclei. The majority of deformed nuclei have axially symmetric shapes with an additional symmetry plane perpendicular to the nuclear symmetry axis. In this section we deal with this kind of nuclei.

A general multipole operator, in the laboratory frame, of order $L$ is related with the intrinsic one through

$$\hat{T}_{LM}(\text{lab}) = \sum_{M'} D_{LM}^{L} T_{LM}'(\text{int}),$$

where $D$ are the rotation matrices. Laboratory and intrinsic states are also related through the $D$ matrices,

$$|JMK, \xi\rangle = \sqrt{\frac{2J+1}{16\pi^2(1+\delta_{K0})}} (D_{MK}^{J} + (-1)^{J+K} D_{MK}^{J} R_{2}(\pi)) |K\xi\rangle,$$

where $\xi$ [cfr. (12)] denotes the intrinsic part of the wave function and $K$ the projection of the total angular momentum on the symmetry axis.

In our case $|K\xi\rangle$ are the intrinsic states [10, 14, 30, 31] and reduced matrix elements in the laboratory frame can be related to the intrinsic matrix elements as follows:

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\[ \langle J K, \xi | T_L(\text{lab}) | J'K', \xi' \rangle = \sqrt{2J' + 1} \left( \langle J'K' LK - K'|JK \rangle \langle K\xi | \hat{T}_{LK-K'}(\text{int}) | K'\xi' \rangle \right) + (-1)^{J' + K'} \langle J' - K' LK + K'|JK \rangle \langle K\xi | \hat{T}_{LK+K'} | K'\xi' \rangle \frac{2}{1 + \delta_{K0} + \delta_{K'0} + \delta_{KK'}}. \]  

(43)

The last factor in r.h.s. is introduced to take into account that our intrinsic states contain both components ±\(K\).

The reduced transition probability for a transition between states belonging to two rotational bands is given by

\[ B(E2, J'K', \xi' \rightarrow JK, \xi) = \frac{1}{2J' + 1} |\langle JK, \xi | T_L(\text{lab}) | J'K', \xi' \rangle|^2. \]  

(44)

The knowledge of the intrinsic matrix element between two rotational bands hence determines the reduced matrix element \(\langle 43\rangle\) from where the reduced transition probability can be deduced.

Of special relevance to Nuclear Physics are \(E2\) transitions and results given in this section are confined to this type of transition. The most general one-body \(E2\) operator is defined in Eq. \(\langle 3\rangle\) (with an effective charge equal to 1). Matrix elements between the ground state and one-phonon states are given in Ref. \[26\]. Likewise, matrix elements between one- and two-phonon can be derived. The non-vanishing ones are given by (we keep the \(\gamma\)-dependence for generality)

\[ \langle \beta | \hat{T}_{20} | \beta \rangle = \frac{(1 - \beta^2) \cos \gamma - \sqrt{2} \beta \chi \cos 2\gamma}{1 + \beta^2}, \]  

(45)

\[ \langle \beta | \hat{T}_{2\pm 2} | \beta \rangle = \frac{1}{\sqrt{2}(N - 1)} \sqrt{2} \left( (1 - \beta^2) \sin \gamma + \frac{1}{\sqrt{2}} \beta \chi \sin 2\gamma \right), \]  

(46)

\[ \langle \beta | \hat{T}_{20} | \beta \gamma_+ \rangle = \sqrt{N - 1} \frac{\sin \gamma + \sqrt{2} \beta \chi \sin 2\gamma}{\sqrt{1 + \beta^2}}, \]  

(47)

\[ \langle \beta | \hat{T}_{2\pm 2} | \beta \gamma_+ \rangle = \sqrt{N - 1} \frac{\cos \gamma + \frac{1}{\sqrt{2}} \beta \chi \cos 2\gamma}{\sqrt{1 + \beta^2}}, \]  

(48)

\[ \langle \gamma_+ | \hat{T}_{20} | \beta \gamma_+ \rangle = \frac{1}{\sqrt{2}} \langle \beta | \hat{T}_{20} | \beta \rangle, \]  

(49)
\begin{align}
\langle \gamma_+ | \hat{T}_{2\pm 2} | \beta \gamma_+ \rangle &= \frac{1}{\sqrt{2}} \langle \beta | \hat{T}_{2\pm 2} | \beta^2 \rangle, \\
\langle \gamma_+ | \hat{T}_{20} | \gamma_{K=0}^2 \rangle &= \langle \gamma_+ | \hat{T}_{20} | \gamma_{K=4}^2 \rangle = \langle \beta | \hat{T}_{20} | \beta \gamma_+ \rangle, \\
\langle \gamma_+ | \hat{T}_{2\pm 2} | \gamma_{K=0}^2 \rangle &= \langle \gamma_+ | \hat{T}_{2\pm 2} | \gamma_{K=4}^2 \rangle = \langle \beta | \hat{T}_{2\pm 2} | \beta \gamma_+ \rangle, \\
\langle \beta^2 | \hat{T}_{20} | \beta^2 \rangle &= (N-2) \frac{2 \beta \cos \gamma - \sqrt{\frac{7}{\beta}} \chi \cos 2\gamma}{1 + \beta^2} + 2 \frac{-2 \beta \cos \gamma - \sqrt{\frac{7}{\beta}} \chi \cos 2\gamma}{1 + \beta^2}, \\
\langle \beta^2 | \hat{T}_{2\pm 2} | \beta^2 \rangle &= (N-2) \frac{\sqrt{2} \beta \sin \gamma + \frac{1}{\sqrt{7}} \beta \chi \sin 2\gamma}{1 + \beta^2} + 2 \frac{-\sqrt{2} \beta \sin \gamma + \frac{1}{\sqrt{7}} \chi \sin 2\gamma}{1 + \beta^2}, \\
\langle \beta^2 | \hat{T}_{20} | \beta \gamma_+ \rangle &= \frac{\sqrt{2} \beta \sin \gamma + \frac{2}{\sqrt{7}} \chi \sin 2\gamma}{\sqrt{1 + \beta^2}}, \\
\langle \beta^2 | \hat{T}_{2\pm 2} | \beta \gamma_+ \rangle &= \frac{-\beta \cos \gamma + \sqrt{\frac{7}{\beta}} \chi \cos 2\gamma}{\sqrt{1 + \beta^2}}, \\
\langle \beta_+ | \hat{T}_{20} | \beta_+ \rangle &= (N-2) \frac{2 \beta \cos \gamma - \sqrt{\frac{7}{\beta}} \beta^2 \chi \cos 2\gamma}{1 + \beta^2} + \frac{-2 \beta \cos \gamma - \sqrt{\frac{7}{\beta}} \chi \cos 2\gamma}{1 + \beta^2} \\
&\quad + \sqrt{\frac{2}{7}} \chi \cos 2\gamma, \\
\langle \beta_+ | \hat{T}_{2\pm 2} | \beta_+ \rangle &= (N-2) \frac{\sqrt{2} \beta \sin \gamma + \frac{1}{\sqrt{7}} \beta^2 \chi \sin 2\gamma}{1 + \beta^2} + \frac{-\sqrt{2} \beta \sin \gamma + \frac{1}{\sqrt{7}} \chi \sin 2\gamma}{1 + \beta^2} \\
&\quad - \frac{\chi \sin 2\gamma}{\sqrt{7}} , \\
\langle \beta_+ | \hat{T}_{20} | \gamma_{K=0}^2 \rangle &= \langle \beta_+ | \hat{T}_{20} | \gamma_{K=4}^2 \rangle = \frac{1}{\sqrt{2}} \langle \beta^2 | \hat{T}_{20} | \beta_+ \rangle, \\
\langle \beta_+ | \hat{T}_{2\pm 2} | \gamma_{K=0}^2 \rangle &= \langle \beta_+ | \hat{T}_{2\pm 2} | \gamma_{K=4}^2 \rangle = \frac{1}{\sqrt{2}} \langle \beta^2 | \hat{T}_{2\pm 2} | \beta_+ \rangle, \\
\langle \gamma_{K=0}^2 | \hat{T}_{20} | \gamma_{K=0}^2 \rangle &= \langle \gamma_{K=4}^2 | \hat{T}_{20} | \gamma_{K=4}^2 \rangle = (N-2) \frac{2 \beta \cos \gamma - \sqrt{\frac{7}{\beta}} \beta^2 \chi \cos 2\gamma}{1 + \beta^2} + \frac{\sqrt{2}}{7} \chi (\cos 2\gamma + 1),
\end{align}
\[
\langle \gamma_K^2 | \hat{T}_{2\pm 2} | \gamma_K^2 \rangle = \langle \gamma_K^2 | \hat{T}_{2\pm 2} | \gamma_K^2 \rangle = (N - 2) \frac{\sqrt{2} \beta \sin \gamma + \sqrt{\frac{1}{2} \beta^2} \chi \sin 2\gamma}{1 + \beta^2} - \sqrt{\frac{1}{2}} \chi \sin 2\gamma.
\]

(62)

In order to see the general behaviour of the calculated transitions, in Fig. 7 we present a calculation for the \(B(E2)\)'s as a function of \(\chi\) for the hamiltonian \(H = \kappa_2 (\hat{T}_2 \cdot \hat{T}_2 - \hat{P}^\dagger \hat{P})\). In (a) the calculation is done directly in the lab system while in (b) the intrinsic wave functions and Eqs. (43-44) are used. The main characteristics of the calculated \(B(E2)\)'s are similar to those obtained in the lab in Ref. [25] although in that case only ground state and one phonon excitations are included.

V. CONCLUSIONS

In this paper a formalism is presented for performing calculations with up to two phonon-excitations in the intrinsic frame. This formalism yields good agreement with exact results and allows an easy interpretation of them. The calculations can be easily extended to include higher multi-phonon excitations and/or higher-order interactions.

From these results it is deduced that for a large number of bosons \(N\) the IBM is a harmonic model even if \(n\)-body interactions are included. A sizeable degree of anharmonicity can be obtained only for a finite number of bosons combined with a three-body term in the hamiltonian. This result points towards a link between triaxiality and anharmonicity in the IBM.

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FIGURES

FIG. 1. Energy levels as a function of the number of bosons $N$ for the $SU(3)$ limit. The hamiltonian $H = k_2 \hat{T}_2 \cdot \hat{T}_2$ is used. Full lines correspond to the intrinsic-frame calculations and dashed lines to the laboratory-frame calculations.

FIG. 2. Energy levels as a function of the number of bosons $N$ for the $O(6)$ limit. The hamiltonian $H = k_0 \hat{P}^\dagger \hat{P}$ is used. Full lines correspond to the intrinsic-frame calculations and dashed lines to the laboratory-frame calculations.

FIG. 3. Energy levels and composition of states as a function of the ratio $-\kappa_0/\kappa_2$ for the hamiltonian $H = \kappa_0 \hat{P}^\dagger \hat{P} + \kappa_2 \hat{T}_2 \cdot \hat{T}_2$, with $\chi = -\sqrt{7}/2$ and $N = 16$ for up to (a) two phonons and (b) one phonon.

FIG. 4. Energy levels and composition of the states as a function of the ratio $-\kappa_4/\kappa_2$ for the hamiltonian $H = \kappa_2 \hat{T}_2 \cdot \hat{T}_2 + \kappa_4 \hat{T}_4 \cdot \hat{T}_4$, with $\chi = -\sqrt{7}/2$ and $N = 16$ for up to (a) two phonons and (b) one phonon.

FIG. 5. Energy levels and composition of the states as a function of the ratio $-\varepsilon_4/\kappa_2$ for the hamiltonian $H = \varepsilon_d \hat{n}_d + \kappa_2 \hat{T}_2 \cdot \hat{T}_2$, with $\chi = -\sqrt{7}/2$ and $N = 16$ for up to (a) two phonons and (b) one phonon.

FIG. 6. Excitation energies and composition of the states as a function of $\gamma$ in a $\gamma$-perturbed mean-field calculation for the hamiltonian $H = \kappa_2 (\hat{T}_2 \cdot \hat{T}_2 - \hat{P}^\dagger \hat{P})$, with $\chi = -\sqrt{7}/2$ and $N = 16$.

FIG. 7. $B(E2)$ values for selected transitions between ground, one- and two-phonon excited states for a hamiltonian $H = \kappa_2 (\hat{T}_2 \cdot \hat{T}_2 - \hat{P}^\dagger \hat{P})$ as a function of $\chi$ for a system with $N = 16$. In (a) the calculation is done directly in the lab system and in (b) the intrinsic wave functions and Eqs. (43-44) are used.
\( -E / \kappa_2 \)

(a) \( 96\% \gamma_{K=0}^2 + 3.96\% \beta^2 \)

(b) \( 78\% \beta + 22\% \gamma_{K=0}^2 \)

\( \beta \gamma \)

\( \gamma_{K=0}^2 \)

\( \gamma_{K=4}^2 \)

\( \beta \gamma \)

\( \gamma \)

\( \beta \)

\( \gamma \)

\( \gamma \)
\[
\frac{(2\chi)^2}{\sqrt{7}}
\]