Electromagnetic transitions in hypothetical tetrahedral and octahedral bands

A. Dobrowolski, A. Szulerecka, A. Góźdź

September 29, 2012

Contents

1. Octahedral quadrupole+octupole collective model
2. Selection rules
3. Symmetrization procedure
4. Construction of symmetrized collective basis states
5. Results: Electric transitions in ^{156}Gd

Group chains for the 32 crystalographic point groups.

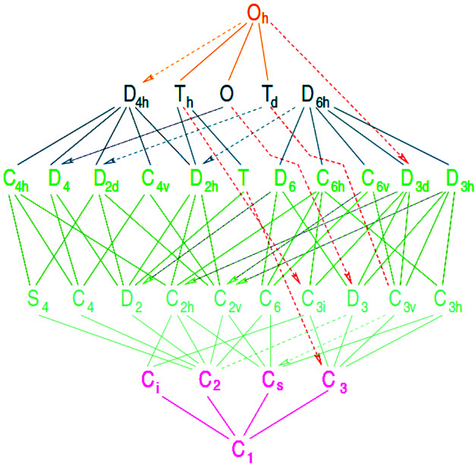


Figure: Koster et al. *Thirty Two Point Groups*, 1963

Degeneracy of energetical levels

Let the Hamiltonian $\hat{H}$ be O_h–symmetric.

Irreducible representations (briefly *irreps*) for the octahedral O/T_d–groups are:
A_1, A_2 – 1-D irreps., E – 2-D irrep., T_1, T_2 – 3-D irreps.

Schematic degenerated spectrum of $\hat{H}$

$T_1;\ \ \psi_1^{T_1}, \psi_2^{T_1}, \psi_3^{T_1}$

$A_1;\ \ \varphi_1^{A_1}$

$A_2;\ \ \psi_1^{A_2}$

$E;\ \ \psi_1^{E}, \psi_2^{E}$

$T_2;\ \ \psi_1^{T_2}, \psi_2^{T_2}, \psi_3^{T_2}$

$A_1;\ \ \psi_1^{A_1}$

Octahedral collective quadrupole+octupole model in the intrinsic frame

We construct our deformed collective model already in the intrinsic frame–contrarly to the usual procedure which starts from the spherical Hamiltonian expressed in laboratory coordinates.

The set of collective variables in the intrinsic coordinate system:

$$\alpha_{20}, \alpha_{22}, \{\alpha_{3\nu}\}, \Omega$$

$\Omega-$ is the set of Euler angles between laboratory and intrinsic frame.

Nuclear surface in the intrinsic coordinate system:

$$R(\theta,\varphi) = R_0[1 + \alpha_{20} Y_{20}(\theta,\varphi) + \alpha_{22}(Y_{22}(\theta,\varphi) + Y_{2,-2}(\theta,\varphi)) + \\ + \sum_{\nu=-3}^{3} \alpha^*_{3\nu} Y_{3\nu}(\theta,\varphi)]$$

Collective solutions

We construct the collective space for a schematic octahedrally-symmetric Hamiltonian invariant also with respect to the symmetrization group O:

$$\hat{H} = \hat{H}_{vib;2} + \hat{H}_{vib;3} + \hat{H}_{rot}$$

In case of no coupling between the 3 components of $\hat{H}$ its eigensolutions are the product of the eigensolutions of individual Hamiltonians

$$\psi(\alpha_2, \alpha_3, \Omega) = \psi^{\Gamma_1}_{vib,2}(\alpha_2)\psi^{\Gamma_2}_{vib,3}(\alpha_3)\psi^{\Gamma_3}_{rot}(\Omega)$$

Each of these 3 functions belongs to only one irrep.Γ_i of the $O-$group.

Construction of the collective space consists in determining basis vectors corresponding to he quadr., oct. and rot. motions

$\psi_{vib,2}(\alpha_2)$ - basis in the space of eigensolutions of $\hat{H}_{vib;2}$,
$\psi_{vib,3}(\alpha_3)$ - basis in the space of eigensolutions of $\hat{H}_{vib;3}$,
$\psi_{rot}(\Omega)$ - basis in the space of eigensolutions of $\hat{H}_{rot}$.

Selection rules for electromagnetic transitions

Suppose that the initial and final states of $\hat{H}$, $|I_1 M_1\rangle, |I_2 M_2\rangle$ belong to the representations Γ^1, Γ^2 respectively and the tensor operator, $\hat{Q}^{lab}_{\lambda\nu}$ transforms with respect to the irrep. Γ^Q.

The matrix element $\langle I_2 M_2|\hat{Q}^{lab}_{\lambda\nu}|I_1 M_1\rangle$ can be non-zero than and only than

$$\Gamma^1 \times \Gamma^Q \supset \Gamma^2$$

Let $|I_1 M_1\rangle$, $|I_2 M_2\rangle$, $\hat{Q}^{lab}_{2\nu}$ belong respectively to irreps. T_1, T_2, E of the O–group.
The Kronecker product $T_1 \times E$ decomposes into the simple sum of two irreps. T_1 and T_2.

Since $|I_2 M_2\rangle$ belongs to irrep. T_2, then such a matrix element can be non-zero

If $|I_2 M_2\rangle$ does not belong to irrep. T_1 or T_2 then such transition is forbidden.

Collective electric transition operators

(Eisenberg, Greiner, Nuclear theory, 1970).

The collective transition operator up to the second order in the laboratory frame:

$$\hat{Q}^{lab}_{\lambda\mu} = \sum_{\nu} D^{\lambda}_{\mu\nu}(\Omega)^{\star}\hat{Q}^{intr}_{\lambda\nu}, \quad \text{where}$$

$$\hat{Q}^{intr}_{\lambda\nu} = \frac{3ZR_0^{\lambda}}{4\pi}\Big\{\alpha_{\lambda\nu} + \frac{\lambda+2}{2\sqrt{4\pi}}\sum_{\lambda_1\lambda_2}\sqrt{\frac{(2\lambda_1+1)(2\lambda_2+1)}{2\lambda+1}} \times$$

$$(\lambda_1 0 \lambda_2 0|\lambda 0)(\alpha_{\lambda_1}\otimes\alpha_{\lambda_2})^{\lambda}_{\nu}\Big\}$$

Collective electric transition operators – examples

The intrinsic frame is chosen to fix quadrupoles in the principal axes frame. There are no extra conditions for octupole variables. The **intrinsic** part of the dipole transition operator:

$$\hat{Q}_{10}^{intr} = \frac{3\sqrt{3}ZR_0}{16\pi\sqrt{\pi}}\Big\{\frac{6}{\sqrt{7}}\alpha_{22}\alpha_{3-2} - 12\sqrt{\frac{2}{35}}\alpha_{21}\alpha_{3-1}$$
$$+\frac{18}{\sqrt{35}}\alpha_{20}\alpha_{30} - 12\sqrt{\frac{2}{35}}\alpha_{2-1}\alpha_{31} + \frac{6}{\sqrt{7}}\alpha_{22}\alpha_{3-2}\Big\}$$

The quadrupole intrinsic operator:

$$\hat{Q}_{20}^{intr} = \frac{3ZR_0^2}{4\pi}\Big\{\alpha_{20}$$
$$+\frac{1}{\sqrt{5\pi}}\Big(\frac{10}{7}\alpha_{20}\alpha_{20} - \frac{20}{7}\alpha_{2-2}\alpha_{22} + \frac{4}{3}\alpha_{30}\alpha_{30} - 2\alpha_{3-1}\alpha_{31} + \frac{10}{3}\alpha_{3-3}\alpha_{33}\Big)$$
$$= \hat{Q}_{20}^{quadr}(1^{st}) + \hat{Q}_{20}^{quadr}(2^{nd}) + \hat{Q}_{20}^{oct}(2^{nd})$$

NO tetrahedral collective variable !!!!!!

Selection rules – other examples

1. Forbidden quadrupole transitions

$$\langle I_2 M_2; A_1 | \hat{Q}^{lab}_{2\nu} | I_1 M_1; A_1 \rangle = 0$$
$$\langle I_2 M_2; A_1 | \hat{Q}^{lab}_{2\nu} | I_1 M_1; A_2 \rangle = 0$$
$$\langle I_2 M_2; A_2 | \hat{Q}^{lab}_{2\nu} | I_1 M_1; A_2 \rangle = 0$$

2. Forbidden dipole transitions

$$\langle I_2 M_2; A_1 | \hat{Q}^{lab}_{1\nu} | I_1 M_1; A_1 \rangle = 0$$
$$\langle I_2 M_2; A_1 | \hat{Q}^{lab}_{1\nu} | I_1 M_1; A_2 \rangle = 0$$
$$\langle I_2 M_2; A_2 | \hat{Q}^{lab}_{1\nu} | I_1 M_1; A_2 \rangle = 0$$

Since $\langle \psi'^{A_1(A_2)}_{vib,2} | \hat{Q}^{quadr}_{2\nu}(1^{st}) | \psi^{A_1(A_2)}_{vib,2} \rangle = 0$ then $B(E2)$ comes only from quadrupole and octupole $2^{nd}-$order operator $\hat{Q}^{quadr}_{20}(2^{nd}) + \hat{Q}^{oct}_{20}(2^{nd})$ (**dynamical deformation effect**)

Relation between intrinsic and laboratory frame

The relation between collective laboratory and intrinsic shape variables

$$\alpha^{lab}_{\lambda\mu}(\alpha_{\lambda\nu}) = \sum_{\nu=-\lambda}^{\lambda} D^{\lambda *}_{\mu\nu}(\Omega)\, \alpha_{\lambda\nu}$$

with additional 3 conditions:

$$f_k(\alpha_{\lambda\mu}, \Omega) = 0, \ \ \{k = 1, 2, 3\},$$

Above conditions determine the orientation of both intrinsic vs laboratory frame.

Intrinsic frame

The transformation from the laboratory to intrinsic coordinate system is, in general, non-reversible.

It means that, for one given set of laboratory variables $\{\alpha_{\lambda\nu}^{lab}\}$ usualy may correspond several sets of intrinsic variables $\{\alpha_{\lambda\mu}, \Omega\}$, (well known problem e.g. for the so called Bohr Hamiltonian)

$$\alpha_{\lambda\nu}^{lab}(\alpha_{\lambda\nu}, \Omega) = \alpha_{\lambda\nu}^{lab}(\alpha_{\lambda\nu}^{'}, \Omega^{'})$$

where $(\alpha_{\lambda\nu}, \Omega) \neq (\alpha_{\lambda\nu}^{'}, \Omega^{'})$

How to omit this disadvantage?

Symmetrization group

It is possible to find the **intrinsic transformation group** of the intrinsic variables which does not change the transformation relation between intrinsic and laboratory variables

$$\alpha^{lab}_{\lambda\nu}(\hat{g}(\alpha_{\lambda\nu},\Omega)) = \alpha^{lab}_{\lambda\nu}(\alpha_{\lambda\nu},\Omega)$$

The set of all transformations $\hat{g}$ forms the so called **symmetrization group** G_s.

Symmetrization - applications

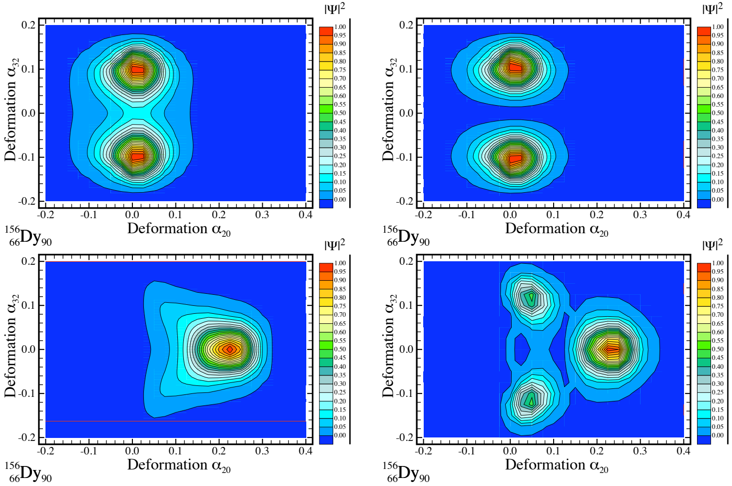
- Suppose that in the laboratory frame we have both the quadrupole $\{\alpha_{2\nu}^{lab}\}$ and octupole variables $\{\alpha_{3\nu}^{lab}\}$
  Three standard conditions determining the intrinsic frame:
  $\alpha_{2\pm1} = 0, \alpha_{22} = \alpha_{2-2}$.
  Intrinsic variables: $\{\alpha_{20}, \alpha_{22}, \alpha_{3\nu}, \Omega\}$.
  Relation between the laboratory and intrinsic frames:

$$\alpha_{2\nu}^{lab} = D_{\nu 0}^{2*}(\Omega)\,\alpha_{20} + [D_{\nu -2}^{2*}(\Omega) + D_{\nu 2}^{2*}(\Omega)]\alpha_{22}$$
$$\nu = 0, \pm1, \pm2$$
$$\alpha_{3\nu}^{lab} = \sum_{\mu=-3}^{3} D_{\nu\mu}^{3*}(\Omega)\,\alpha_{3\mu}$$
$$\nu = 0, \pm1, \pm2, \pm3$$

Solving this set of equations one gets the symmetrization group, $G_s = O$

Four possible types of solutions of the ATDHF 2-D quadr.+oct. Hamiltonian (IJMP E, vol.20, 2011, p. 500-505)

$|\Psi_{vib}|^2$ as function of α_{20} and $\alpha"_{32}$ for ^{156}Dy.



Quadrupole basis states

More realistic multidimensional collective quadrupole+octupole Hamiltonian can be diagonalized in a "symmetrized" basis which can be constructed as shown in the following.

The vibrational quadrupole functions of a given O-group irrep. are obtained using the projecting onto a given irrep. method applied for the "shifted" zero- and one-phonon H.O. eigensolutions

$$f(\eta_2, \alpha_{20}, \alpha_{22}) = u_n(\eta_2, \alpha_{20} - \overset{\circ}{\alpha}_{20}) u_m(\sqrt{2}\eta_2, \alpha_{22} - \overset{\circ}{\alpha}_{22})$$

where $\overset{\circ}{\alpha}_{20}$, $\overset{\circ}{\alpha}_{22}$, η_2 are parameters denoting respectively the position of the wave-function peak in α_{20} and α_{22} direction and its "width".
Now we consider only 3 lowest basis states: $\{n = 0, m = 0\}$ or $\{n = 1, m = 0\}$ or $\{n = 0, m = 1\}$.

Resulting (projected) quadrupole functions belong to irreps. A_1, A_2, E

Quadrupole basis states – example

Quadrupole (A_1) state projected out from $u_0(\alpha_{20} - \mathring{\alpha}_{20}) u_0(\alpha_{22} - \mathring{\alpha}_{22})$

$$\Psi_{A1}(\alpha_{20}, \alpha_{22}) = \mathcal{N}_{A_1} \times$$

$$\Big\{ u_0\Big(\eta_2; \alpha_{20} + \frac{1}{2}(\mathring{\alpha}_{20} + \sqrt{6}\,\mathring{\alpha}_{22})\Big) u_0\Big(\sqrt{2}\eta_2; \alpha_{22} + \frac{1}{4}(\sqrt{6}\,\mathring{\alpha}_{20} - 2\,\mathring{\alpha}_{22})\Big)$$

$$+ u_0\Big(\eta_2; \alpha_{20} + \frac{1}{2}(\mathring{\alpha}_{20} + \sqrt{6}\,\mathring{\alpha}_{22})\Big) u_0\Big(\sqrt{2}\eta_2; \alpha_{22} - \frac{1}{4}(\sqrt{6}\,\mathring{\alpha}_{20} - 2\,\mathring{\alpha}_{22})\Big)$$

$$+ u_0\Big(\eta_2; \alpha_{20} + \frac{1}{2}(\mathring{\alpha}_{20} - \sqrt{6}\,\mathring{\alpha}_{22})\Big) u_0\Big(\sqrt{2}\eta_2; \alpha_{22} + \frac{1}{4}(\sqrt{6}\,\mathring{\alpha}_{20} + 2\,\mathring{\alpha}_{22})\Big)$$

$$+ u_0\Big(\eta_2; \alpha_{20} + \frac{1}{2}(\mathring{\alpha}_{20} - \sqrt{6}\,\mathring{\alpha}_{22})\Big) u_0\Big(\sqrt{2}\eta_2; \alpha_{22} - \frac{1}{4}(\sqrt{6}\,\mathring{\alpha}_{20} + 2\,\mathring{\alpha}_{22})\Big) +$$

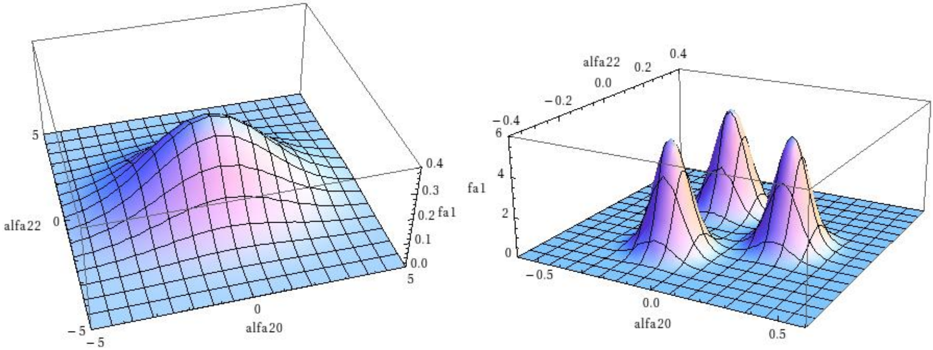
$$u_0\Big(\eta_2; \alpha_{20} - \mathring{\alpha}_{20}\Big) u_0\Big(\sqrt{2}\eta_2; \alpha_{22} - \mathring{\alpha}_{22}\Big) + u_0\Big(\eta_2; \alpha_{20} - \mathring{\alpha}_{20}\Big) u_0\Big(\sqrt{2}\eta_2; \alpha_{22} + \mathring{\alpha}_{22}\Big) \Big\}$$

Important features:

$$\langle A_1 | \hat{\alpha}_{20} | A_1 \rangle = \langle A_1 | \hat{\alpha}_{22} | A_1 \rangle = 0$$

$$\langle A_1 | \hat{\alpha}_{20}^2 | A_1 \rangle \neq 0, \quad \langle A_1 | \hat{\alpha}_{22}^2 | A_1 \rangle \neq 0 \quad \propto \mathcal{A}^2(\alpha_{2\nu}) \propto 1/\eta^2$$

ψ_{A_1} state as function of α_{20} and α_{22}



Left panel: $\mathring{\alpha}_{20} = 0.26$, $\mathring{\alpha}_{22} = 0.02$, $\eta_2 = 0.5$
Right panel: $\mathring{\alpha}_{20} = 0.26$, $\mathring{\alpha}_{22} = 0.02$, $\eta_2 = 15$

Octupole basis states

The projected vibrational octupole **one-phonon** functions are the linear combinations of 7-D oscillator solutions

$$f(\eta_3, \{\alpha_{3\mu}\}) = u_{n_1}(\eta_3, \alpha^r_{30}) u_{n_2}(\eta_3, \alpha^r_{31}) u_{n_3}(\eta_3, \alpha^r_{32}) u_{n_4}(\eta_3, \alpha^r_{33})$$
$$u_{n_5}(\eta_3, \alpha^i_{31}) u_{n_6}(\eta_3, \alpha^i_{32} \pm \overset{\circ}{\alpha}{}^i_{32}) u_{n_7}(\eta_3, \alpha^i_{33})$$

(r-real, i-imaginary parts of $\alpha_{3\mu}$), $n_k = 0, 1$ and $\sum n_k = 1$.

The resulting projected functions belong to the following irreps.

(a) A_1, T_1, T_2 – positive parity functions

(b) A_2, T_1, T_2 – negative parity functions

No E irreducible representation in ocupoles

Example: T_1 negative-parity octupole state

Triplet transforming with respect to irrep. T_1

$$\psi_{T_{1,1}}(\alpha_{3\nu}) = \mathcal{N} u_1(\eta_3;\alpha_{30}) u_0(\sqrt{2}\eta_3;\alpha'_{31}) u_0(\sqrt{2}\eta_3;\alpha'_{32})$$
$$u_0(\sqrt{2}\eta_3;\alpha'_{33}) u_0(\sqrt{2}\eta_3;\alpha"_{31}) u_0(\sqrt{2}\eta_3;\alpha"_{33})$$
$$\{u_0(\sqrt{2}\eta_3;\alpha"_{32} - \mathring{\alpha}"_{32}) + u_0(\sqrt{2}\eta_3;\alpha"_{32} + \mathring{\alpha}"_{32})\}$$

$$\psi_{T_{1,2}}(\alpha_{3\nu}) = \mathcal{N}' u_0(\eta_3;\alpha_{30}) u_0(\sqrt{2}\eta_3;\alpha'_{32}) u_0(\sqrt{2}\eta_3;\alpha"_{31}) u_0(\sqrt{2}\eta_3;\alpha"_{33})$$
$$\{u_0(\sqrt{2}\eta_3;\alpha"_{32} - \mathring{\alpha}"_{32}) + u_0(\sqrt{2}\eta_3;\alpha"_{32} + \mathring{\alpha}"_{32})\}$$
$$\{\sqrt{5} u_0(\sqrt{2}\eta_3;\alpha'_{31}) u_1(\sqrt{2}\eta_3;\alpha'_{33}) - \sqrt{3} u_1(\sqrt{2}\eta_3;\alpha'_{31}) u_0(\sqrt{2}\eta_3;\alpha'_{33})\}$$

$$\psi_{T_{1,3}}(\alpha_{3\nu}) = \mathcal{N}'' u_0(\eta_3;\alpha_{30}) u_0(\sqrt{2}\eta_3;\alpha'_{31}) u_0(\sqrt{2}\eta_3;\alpha'_{32}) u_0(\sqrt{2}\eta_3;\alpha'_{33})$$
$$\{u_0(\sqrt{2}\eta_3;\alpha"_{32} - \mathring{\alpha}"_{32}) + u_0(\sqrt{2}\eta_3;\alpha"_{32} + \mathring{\alpha}"_{32})\}$$
$$\{\sqrt{3} u_1(\sqrt{2}\eta_3;\alpha"_{31}) u_0(\sqrt{2}\eta_3;\alpha"_{33}) + \sqrt{5} u_0(\sqrt{2}\eta_3;\alpha"_{31}) u_1(\sqrt{2}\eta_3;\alpha"_{33})\}$$

Example: T_2 negative-parity octupole state

Triplet transforming with respect to irrep. T_2

$$\psi_{T_{2,1}}(\alpha_{3\nu}) = \mathcal{N} u_0(\eta_3; \alpha_{30}) u_0(\sqrt{2}\eta_3; \alpha'_{31}) u_1(\sqrt{2}\eta_3; \alpha'_{32}) u_0(\sqrt{2}\eta_3; \alpha'_{33}) u_0(\sqrt{2}\eta_3; \alpha''_{31}) u_0(\sqrt{2}\eta_3; \alpha''_{33}) \{u_0(\sqrt{2}\eta_3; \alpha''_{32} - \mathring{\alpha}''_{32}) + u_0(\sqrt{2}\eta_3; \alpha''_{32} + \mathring{\alpha}''_{32})\}$$

$$\psi_{T_{2,2}}(\alpha_{3\nu}) = \mathcal{N}' u_0(\eta_3; \alpha_{30}) u_0(\sqrt{2}\eta_3; \alpha'_{32}) u_0(\sqrt{2}\eta_3; \alpha''_{31}) u_0(\sqrt{2}\eta_3; \alpha''_{33}) \{u_0(\sqrt{2}\eta_3; \alpha''_{32} - \mathring{\alpha}''_{32}) + u_0(\sqrt{2}\eta_3; \alpha''_{32} + \mathring{\alpha}''_{32})\} \{\sqrt{5} u_1(\sqrt{2}\eta_3; \alpha'_{31}) u_0(\sqrt{2}\eta_3; \alpha'_{33}) + \sqrt{3} u_0(\sqrt{2}\eta_3; \alpha'_{31}) u_1(\sqrt{2}\eta_3; \alpha'_{33})\}$$

$$\psi_{T_{2,3}}(\alpha_{3\nu}) = \mathcal{N}'' u_0(\eta_3; \alpha_{30}) u_0(\sqrt{2}\eta_3; \alpha'_{31}) u_0(\sqrt{2}\eta_3; \alpha'_{32}) u_0(\sqrt{2}\eta_3; \alpha'_{33}) \{u_0(\sqrt{2}\eta_3; \alpha''_{32} - \mathring{\alpha}''_{32}) + u_0(\sqrt{2}\eta_3; \alpha''_{32} + \mathring{\alpha}''_{32})\} \{\sqrt{3} u_0(\sqrt{2}\eta_3; \alpha''_{31}) u_1(\sqrt{2}\eta_3; \alpha''_{33}) - \sqrt{5} u_1(\sqrt{2}\eta_3; \alpha''_{31}) u_0(\sqrt{2}\eta_3; \alpha''_{33})\}$$

IMPORTANT:

For the octupole T_1 state (with possible spins $J = 1, 3, 4, 5, ...$) the axial octupole mode α_{30} is excited.

while

For the octupole T_2 state (with possible spins $J = 2, 3, 4, 5, ...$) the tetrahedral mode α_{32}" is excited.

CONCLUSION:
If T_1 states are preferable as vibrational band-heads, the octupole band should start from $J = 1^-$, otherwise, $J = 3^-$ is the lowest octupole state

Rotational basis

Rotational functions of given J are obtained by projecting linear combinations of the Wigner functions $D^{J*}_{\mu\nu}(\Omega)$ onto the irreps. of the O–group

Resulting functions can belong to all possible irreps. of the $O-$group A_1, A_2, E, T_1 or T_2, depending on the spin J.

Basis of $O-$group built of rotational functions

Example of rotational functions for $J = 0, 1$

$$
\begin{aligned}
r^J_{MK}(\Omega) &= \sqrt{2J+1} D^J_{MK}(\Omega)^* \\
r^{(+)J}_{MK}(\Omega) &= \frac{1}{\sqrt{2(1+\delta_{K0})}}(r^J_{MK} + r^J_{M-K}), K \geq 0 \\
r^{(-)J}_{MK}(\Omega) &= \frac{1}{\sqrt{2}}(r^J_{MK} - r^J_{M-K}), K > 0
\end{aligned}
$$

$R^{J\ M}_{A\ B}(\Omega)$, A- irrep. of $O-$group, B-irrep. of D_2-group.

$$
J = 0, \quad R^{J=0M=0}_{A1A1K=0}(\Omega) = r^{(+)0}_{00}(\Omega)
$$

$$
J = 1, \quad \begin{cases}
R^{J=1M}_{T1A1K=0}(\Omega) = r^{(+)1}_{M0}(\Omega) \\
R^{J=1M}_{T1B1K=1}(\Omega) = r^{(-)1}_{M1}(\Omega) \\
R^{J=1M}_{T1B3K=1}(\Omega) = r^{(+)1}_{M1}(\Omega)
\end{cases}
$$

Collective motions vs O–group irreps.

Each of above discussed basis functions describing the corresponding collective motion belongs to only one irrep. of O–group

(i) quadrupole vibrations:
possible irrep. A_1, A_2, E

(ii) octupole vibrations:

(a) positive parity states
possible irrep. A_1, T_1, T_2

(b) negative parity states
possible irrep. A_2, T_1, T_2

(iii) rotational motion:

$J = 0$: possible irrep. A_1
$J = 1$: possible irrep. T_1
$J = 2$: possible irrep. E, T_2
$J = 3$: possible irrep. A_2, T_1, T_2
$J = 4$: irrep. A_1, E, T_1, T_2
$J = 5$: irrep. E, $T_{1,1}$, $T_{1,2}$, T_2

Quadrupole+octupole model with quadrupole deformation of the octupole band equal to zero

Let us discuss two rotational bands: the GS band and the lowest octupole negative-parity band (**with zero quadrupole deformation**)

Full symmetrized wave functions of these octupole states are:

$$\Psi = \psi_{vib,2}^{\Gamma_1} \psi_{vib,3}^{\Gamma_2} \psi_{rot}^{\Gamma_3}$$

The only possibility for $\psi_{vib,2}$ in this case is $\psi_{vib,2}^{A_1}$ function ($\Gamma_1 = A_1$)

GS band	negative-parity band
	9^-
8^+	7^-
6^+	5^-
4^+	3^-
2^+	$\mathring{\alpha}_{20}, \mathring{\alpha}_{22} = 0$
0^+	$\mathring{\alpha}_{32} \neq 0$
$\mathring{\alpha}_{20}, \mathring{\alpha}_{22} \neq 0, \mathring{\alpha}_{3\mu} = 0$	$T_d/O-$group
$D_{2h}-$group	

Symmetrized basis functions

Possible products of the basis functions $\psi^{\Gamma_1}_{vib,2}\psi^{\Gamma_2}_{vib,3}\psi^{\Gamma_3}_{rot}$ giving the symmetrized functions with respect to the symmetrization group O

(i) positive parity quadrupole GS functions, (2 cases)

$$\Gamma_1 = A_1, \Gamma_2 = A_1, \Gamma_3 = A_1 \quad J = 0, 4$$
$$\Gamma_1 = E, \Gamma_2 = A_1, \Gamma_3 = E \quad J = 2, 4$$

(ii) negative parity octupole functions, (3 cases)

$$\Gamma_1 = A_1, \Gamma_2 = A_2, \Gamma_3 = A_2 \quad J = 3\ (\mathrm{no\,E1\,transitions})$$
$$\Gamma_1 = A_1, \Gamma_2 = T_1, \Gamma_3 = T_1 \quad J = 1, 3, 4, 5$$
$$\Gamma_1 = A_1, \Gamma_2 = T_2, \Gamma_3 = T_2 \quad J = 2, 3, 4, 5$$

For **octupole** states exp. $B(E1)'$s and $B(E2)'$s in ^{156}Gd are well reproduced within the scheme:
$\Gamma_1 = A_1, \Gamma_2 = T_1, \Gamma_3 = T_1,$ (available $J = 1, 3, 4, 5$).
For the above 3 states, due to mentioned selection rules, $B(E2)'$s are

Results

Quadrupole GS vibrational band-heads obtained out of the 2-D zero- and one-phonon H.O. solutions:

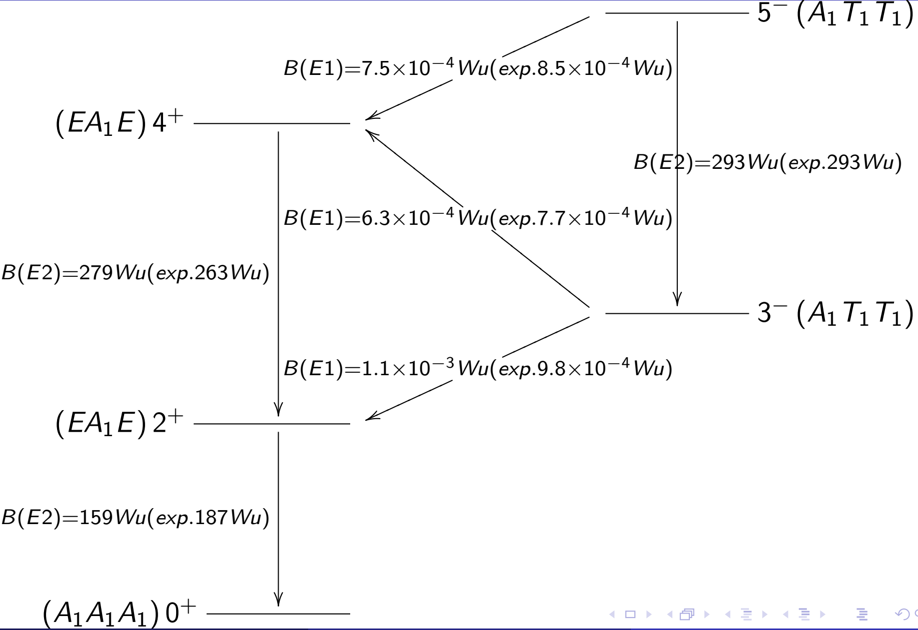
$$0^+ \longrightarrow \text{projected out from } u_0(\alpha_{20} - \overset{\circ}{\alpha}_{20}) u_0(\alpha_{22} - \overset{\circ}{\alpha}_{22})$$
$$2^+ \longrightarrow \text{projected out from } u_0(\alpha_{20} - \overset{\circ}{\alpha}_{20}) u_1(\alpha_{22} - \overset{\circ}{\alpha}_{22})$$
$$4^+ \longrightarrow \text{projected out from } u_0(\alpha_{20} - \overset{\circ}{\alpha}_{20}) u_1(\alpha_{22} - \overset{\circ}{\alpha}_{22})$$

Octupole negative-parity vibrational band-heads are projected out from one-phonon 7-D H.O. solution of the following form:

$$f(\eta_3, \{\alpha_{3\mu}\}) = u_{n_1}(\eta_3, \alpha^r_{30}) u_{n_2}(\eta_3, \alpha^r_{31}) u_{n_3}(\eta_3, \alpha^r_{32}) u_{n_4}(\eta_3, \alpha^r_{33})$$
$$u_{n_5}(\eta_3, \alpha^i_{31}) u_{n_6}(\eta_3, \alpha^i_{32} \pm \overset{\circ}{\alpha}{}^{i}_{32}) u_{n_7}(\eta_3, \alpha^i_{33})$$

(r-real, i-imaginary parts of $\alpha_{3\mu}$), $n_k = 0, 1$ and $\sum n_k = 1$.

Reproducing $B(E1)$ and $B(E2)$ probabilities in ^{156}Gd



Results – parameters of the quadrupole and octupole states

The parameters of the quadrupole and octupole functions are obtained by adjusting the $B(E1)$ and $B(E2)$ probabilities calculated within the above quadrupole and octupole states to its experimental values for ^{156}Gd (*M. Jentschel et al., Phys. Rev. Lett. 222502, (2010)*)

$$\eta_\lambda = \sqrt{\frac{B_\lambda \omega_\lambda}{\hbar}}$$

$$\eta_2 = 12.67$$
$$\eta_{\mathbf{3}} = \mathbf{1.00}$$
$$r_0 = 1.41\ fm$$
$$\overset{\circ}{\alpha}_{22} = 10^{-5}$$
$$\overset{\circ}{\alpha}_{20} = 0.34$$

Quadrupole deformation $\beta_2 = 0.34$.

Quadrupole+octupole model with non-zero quadrupole deformation of the octupole band

GS band

8^+

6^+

4^+

2^+

0^+

$\mathring{\alpha}_{20}, \mathring{\alpha}_{22} \neq 0, \alpha_{3\mu} = 0$

D_{2h}

negative-parity band

9^-

7^-

5^-

3^-

$\mathring{\alpha}_{20}, \mathring{\alpha}_{22} \neq 0$

$\mathring{\alpha}_{32} \neq 0$

T_d / O

IMPORTANT: Symmetrized octupole tetrahedral/octahedral states can have non – zero quadrupole deformation

Symmetrized basis functions

Possible products of the basis functions

$$\Psi = \psi^{\Gamma_1}_{vib,2}\psi^{\Gamma_2}_{vib,3}\psi^{\Gamma_3}_{rot}$$

giving the $O-$symmetrized states

For the quadrupole GS one has 2 possibilities:

$$\Gamma_1 = A_1, \Gamma_2 = A_1, \Gamma_3 = A_1 \quad J = 0, 4$$

$$\Gamma_1 = E, \Gamma_2 = A_1, \Gamma_3 = E \quad J = 2, 4$$

and for the negative parity octupole states built on $\Gamma_1 = E$, with the static deformation $\langle \hat{\alpha}_{2\mu} \rangle \neq 0$ one has 5 possibilities:

$$\Gamma_1 = E, \Gamma_2 = A_2, \Gamma_3 = E \quad J = 2, 4, 5$$

$$\Gamma_1 = E, \Gamma_2 = T_1, \Gamma_3 = T_1 \quad J = 1, 3, 4, 5$$

$$\Gamma_1 = E, \Gamma_2 = T_1, \Gamma_3 = T_2 \quad J = 2, 3, 4, 5$$

$$\Gamma_1 = E, \Gamma_2 = T_2, \Gamma_3 = T_1 \quad J = 1, 3, 4, 5$$

$$\Gamma_1 = E, \Gamma_2 = T_2, \Gamma_3 = T_2 \quad J = 2, 3, 4, 5$$

Symmetrized negative-parity basis functions

For the negative-parity octupole states built on $\Gamma_1 = A_1/A_2$, with static deformation $\langle \hat{\alpha}_{2\mu} \rangle = 0$ we have following 6 possibilities:

$$\Gamma_1 = A_1, \Gamma_2 = A_2, \Gamma_3 = A_2 \quad J = 3$$
$$\Gamma_1 = A_1, \Gamma_2 = T_1, \Gamma_3 = T_1 \quad J = 1, 3, 4, 5$$
$$\Gamma_1 = A_1, \Gamma_2 = T_2, \Gamma_3 = T_2 \quad J = 2, 3, 4, 5$$
$$\Gamma_1 = A_2, \Gamma_2 = A_2, \Gamma_3 = A_1 \quad J = 0, 4$$
$$\Gamma_1 = A_2, \Gamma_2 = T_1, \Gamma_3 = T_2 \quad J = 2, 3, 4, 5$$
$$\Gamma_1 = A_2, \Gamma_2 = T_2, \Gamma_3 = T_1 \quad J = 1, 3, 4, 5$$

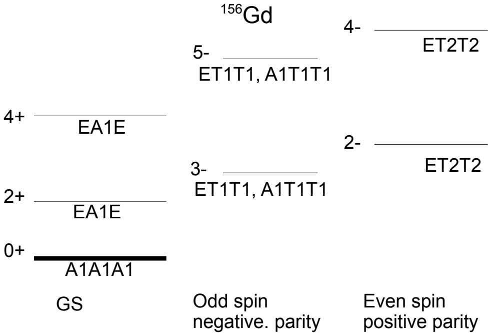
One should study all the 11 combinations of representations $\Gamma_1, \Gamma_2, \Gamma_3$ to find the best reproducing of experimental $BE(1)'$s and $BE(2)'$s
IMPORTANT:
Because of mentioned selection rules a hypothetical band based on above 6 states could have intra-band $B(E2)'$s only due to "dynamical deformation" effects.

Results – parameters of the quadrupole and octupole states

As before, the parameters of the quadrupole and octupole states are adjusted to experimental values of $B(E1)'$s and $B(E2)'$s for ^{156}Gd: (*M. Jentschel et al., Phys. Rev. Lett. 222502, (2010)*)

$$\eta_2 = 12.67$$
$$\eta_3 = 11.60$$
$$r_0 = 1.41\ fm$$
$$\overset{\circ}{\alpha}_{22} = 10^{-5}$$
$$\overset{\circ}{\alpha}{}_{20}^{quadr} = \overset{\circ}{\alpha}{}_{20}^{oct} = 0.34$$

Quadrupole deformation $\beta_2 = 0.34$.



B(E2,4- -->2-)=69.6 W.U.

B(E2,ET1T1,5- -->ET1T1,3-)=176.4 W.U.

B(E2,ET1T1,5- $\rightarrow$ A1T1T1,3-)=342.8 W.U.

B(E2,A1T1T1,5- $\rightarrow$ET1T1,3-)=342.8 W.U.

B(E1,3- -->2+)/B(E1,4- -->4+) ϵ (4,8)

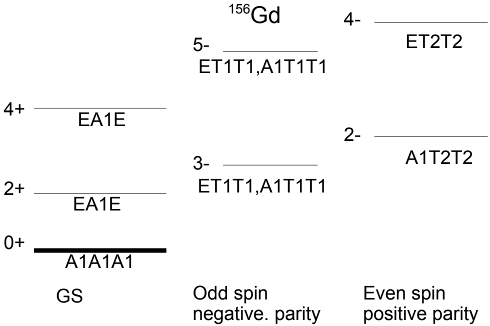
B(E1,3- -->4+)/B(E1,4- -->4+) ϵ (2,4)

B(E1,5- -->4+)/B(E1,4- -->4+) ϵ (2,3)

B(E1,3- -->2+)/B(E1,2- -->2+) ϵ (1,2)

B(E1,3- -->4+)/B(E1,2- -->2+) ϵ (0.6,1)

B(E1,5- -->4+)/B(E1,2- -->2+) ϵ (0.5,1)



B(E2,4- -->2-)=134.7 W.U.

B(E2,ET1T1,5- -->ET1T1,3-)=176.4 W.U.

B(E2,ET1T1,5- → A1T1T1,3-)=342.8 W.U.

B(E2,A1T1T1,5- →ET1T1,3-)=342.8 W.U.

B(E1,3- -->2+)/B(E1,4- -->4+) ϵ (4,8)

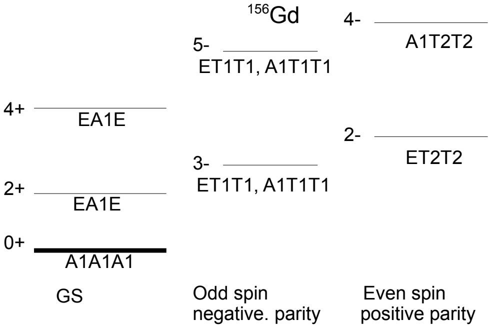
B(E1,3- -->4+)/B(E1,4- -->4+) ϵ (2,4)

B(E1,5- -->4+)/B(E1,4- -->4+) ϵ (2,3)

B(E1,3- -->2+)/B(E1,2- -->2+) ϵ (0.6,1)

B(E1,3- -->4+)/B(E1,2- -->2+) ϵ (0.3,0.7)

B(E1,5- -->4+)/B(E1,2- -->2+) ϵ (0.3,0.5)



B(E2,4- -->2-)=134.7 W.U.

B(E2,ET1T1,5- -->ET1T1,3-)=176.4 W.U.

B(E2,ET1T1,5- → A1T1T1,3-)=342.8 W.U.

B(E2,A1T1T1,5- →ET1T1,3-)=342.8 W.U.

B(E1,3- -->2+)/B(E1,4- -->4+) ϵ (2,4)

B(E1,3- -->4+)/B(E1,4- -->4+) ϵ (1,2)

B(E1,5- -->4+)/B(E1,4- -->4+) ϵ (1,2)

B(E1,3- -->2+)/B(E1,2- -->2+) ϵ (1,2)

B(E1,3- -->4+)/B(E1,2- -->2+) ϵ (0.6,1)

B(E1,5- -->4+)/B(E1,2- -->2+) ϵ (0.5,1)

Symmetrized functions–examples

Examples of symmetrized functions:

1. $\Gamma_1 = A_1, \Gamma_2 = A_1, \Gamma_3 = A_1$ (Ground state)

$$\psi^{A_1}_{vib,2;x^2+y^2+z^2}\psi^{A_1}_{vib,3;x^2+y^2+z^2}\psi^{A_1}_{rot;x^2+y^2+z^2}$$

2. $\Gamma_1 = E, \Gamma_2 = T_2, \Gamma_3 = T_2$ (the most complicated case)

$$\frac{1}{2}\psi^{E}_{vib,2;\sqrt{3}(x^2-y^2)}\psi^{T_2}_{vib,3;yz}\psi^{T_2}_{rot;yz} - \frac{1}{2}\psi^{E}_{vib,2;\sqrt{3}(x^2-y^2)}\psi^{T_2}_{vib,3;xz}\psi^{T_2}_{rot;xz}$$
$$-\frac{\sqrt{3}}{6}\psi^{E}_{vib,2;2z^2-x^2-y^2}\psi^{T_2}_{vib,3;yz}\psi^{T_2}_{rot;yz} - \frac{\sqrt{3}}{6}\psi^{E}_{vib,2;2z^2-x^2-y^2}\psi^{T_2}_{vib,3;xz}\psi^{T_2}_{rot;xz}$$
$$+\frac{\sqrt{3}}{3}\psi^{E}_{vib,2;2z^2-x^2-y^2}\psi^{T_2}_{vib,3;xy}\psi^{T_2}_{rot;xy}$$

Summary

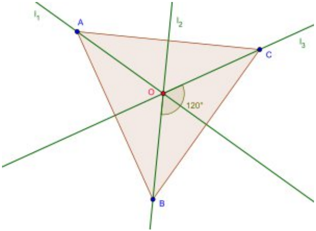
- In the following we have discussed a schematic Hamiltonian with no coupling between quadrupole, octupole and rotational modes,
- Starting from the shifted H.O. eigensolutions we have constructed by the projecting method the symmetrized quadrupole and octupole octahedral/tetrahedral basis states for nuclear spins $J = 0, 1, 2, 3, 4, 5$,
- Using carefully selected only **two** lowest basis states as vibrational band-heads for quadrupole and octupole bands we are able to reproduce with a reasonable accuracy the experimental $B(E1)'$s and $B(E2)'$s in ^{156}Gd up to J=5 ,
- The above presented model reasonably predicts the experimental ratios $B(E1, 5^- \to 4^+)/B(E1, 4^- \to 4^+)$ and $B(E1, 3^- \to 2^+)/B(E1, 2^- \to 2^+)$ in ^{156}Gd,

Point group

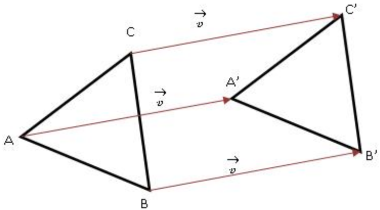
Point group

is a transformation group which keeps at least one point of a figure unchanged.

Rotation about $\frac{2}{3}\pi$, around the perpendicular to the triangle edge axis does not move the point O.



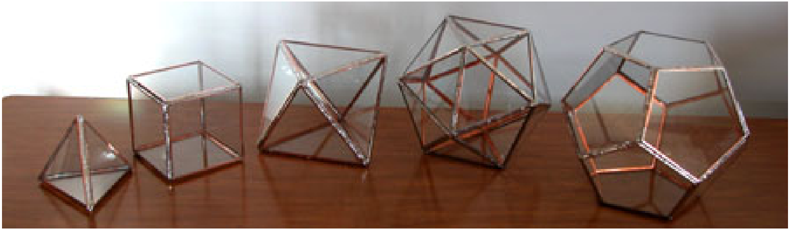
Translation by vector $\vec{v}$ – does not belong to a point group



Grupy punktowe-przykład

Point group as symmetries of Platon figures

1. tetraedron
2. heksaedron
3. oktaedron
4. dodekaedron
5. ikosaedron



Symmetry Group of Hamiltonian

Symmetry Group G of Hamiltonian H is the set of transformations which do not change its shape

With each element of the symmetry group $g \in G$ one can uniquely assign the operator $\hat{g}$

$$\hat{g} H \hat{g}^{-1} = H$$

The eigen-problem of the Hamiltonian H

$$H\psi_{nk} = \epsilon_n \psi_{nk}$$

where ψ_{nk} and ϵ_n are respectively sets of eigenfunctions and eigenenergies of H

Let G be the symmetry group of Hamiltonian H and $g \in G$.

Function $\hat{g}\psi_{nk}$ fulfills the Schrödinger equation for the same

Classifications of the eigenfunctions

Each function $\hat{g}\psi_{nk}$ can be written as the linear combination of ψ_{nk} as:

$$\hat{g}\psi_{nk} = \sum_{k'} \Gamma_{k'k}(g)\psi_{nk'}$$

where $\Gamma(g)$ is the matrix corresponding to $g \in G$.

Set of matrices $\Gamma(g)$ for $g \in G$ is called the group representation while vectors ψ_{nk}– basis of this representation.

Irreducible representations

For unitary representations one can always find such a special transformation of ψ_{nk} basis which transform $\Gamma(g)$ matrices to the block-diagonal form

$$\Gamma(g) = \left(\begin{array}{c|c|c|c} \Gamma^1(g) & 0 & \cdots & 0 \\ \hline 0 & \Gamma^2(g) & \cdots & 0 \\ \hline 0 & 0 & \ddots & 0 \\ \hline 0 & 0 & \cdots & \Gamma^k(g) \end{array}\right)$$

Matrix $\Gamma^i(g)$, $i = 1, 2, \ldots, k$, is called irreducible representation when it is no longer possible to decompose it into block-diagonal form

Kronecker product of reprezentations

Let $\Gamma^1(g), \Gamma^2(g)$ be the reprezentations of group G of ν, μ dimensions respectively.

Kronecker product of reprezentations $\Gamma^1(g), \Gamma^2(g)$ is the following matrix of dimension $\nu\mu$:

$$\Gamma^1(g) \times \Gamma^2(g) = \begin{pmatrix} \Gamma^1_{11}\Gamma^2 & \Gamma^1_{12}\Gamma^2 & \cdots & \Gamma^1_{1\nu}\Gamma^2 \\ \Gamma^1_{21}\Gamma^2 & \Gamma^1_{22}\Gamma^2 & \cdots & \Gamma^1_{2\nu}\Gamma^2 \\ \vdots & \vdots & \ddots & \vdots \\ \Gamma^1_{\nu 1}\Gamma^2 & \Gamma^1_{\nu 2}\Gamma^2 & \cdots & \Gamma^1_{\nu\nu}\Gamma^2 \end{pmatrix}$$

Selection rules for electric transitions

Selection rules for electromagnetic transitions.

Transition probability of $E2$ is proportional to the reduced probability $B(E2)$ given as

$$B(E2; I_1 \rightarrow I_2) = \sum_{M_2,\nu} |\langle I_2 M_2 | M(E2,\nu) | I_1 M_1 \rangle|^2$$

where $|I_1 M_1\rangle, |I_2 M_2\rangle$ are the initial and final states respectively, $M(E2,\nu)$ is the quadrupole electric transitions operator (tensor)

Symmetrization - applications

(ii) Conditions determining the intrinsic frame: $\alpha_{2\pm2} = 0, \alpha_{21} = -\alpha_{2-1}$.
Intrinsic variables: $\{\alpha_{20}, \alpha_{21}, \Omega\}$.
Relation between the laboratory and intrinsic frames:

$$\alpha_{2\nu}^{lab} = D_{\nu 0}^{2*}(\Omega)\,\alpha_{20} + [-D_{\nu -1}^{2*}(\Omega) + D_{\nu 1}^{2*}(\Omega)]\alpha_{21}$$
$$\nu = 0, \pm1, \pm2$$

Symmetrization group $G_s = D_{2h}$