Modeling low-energy states with generalized Bohr Hamiltonian

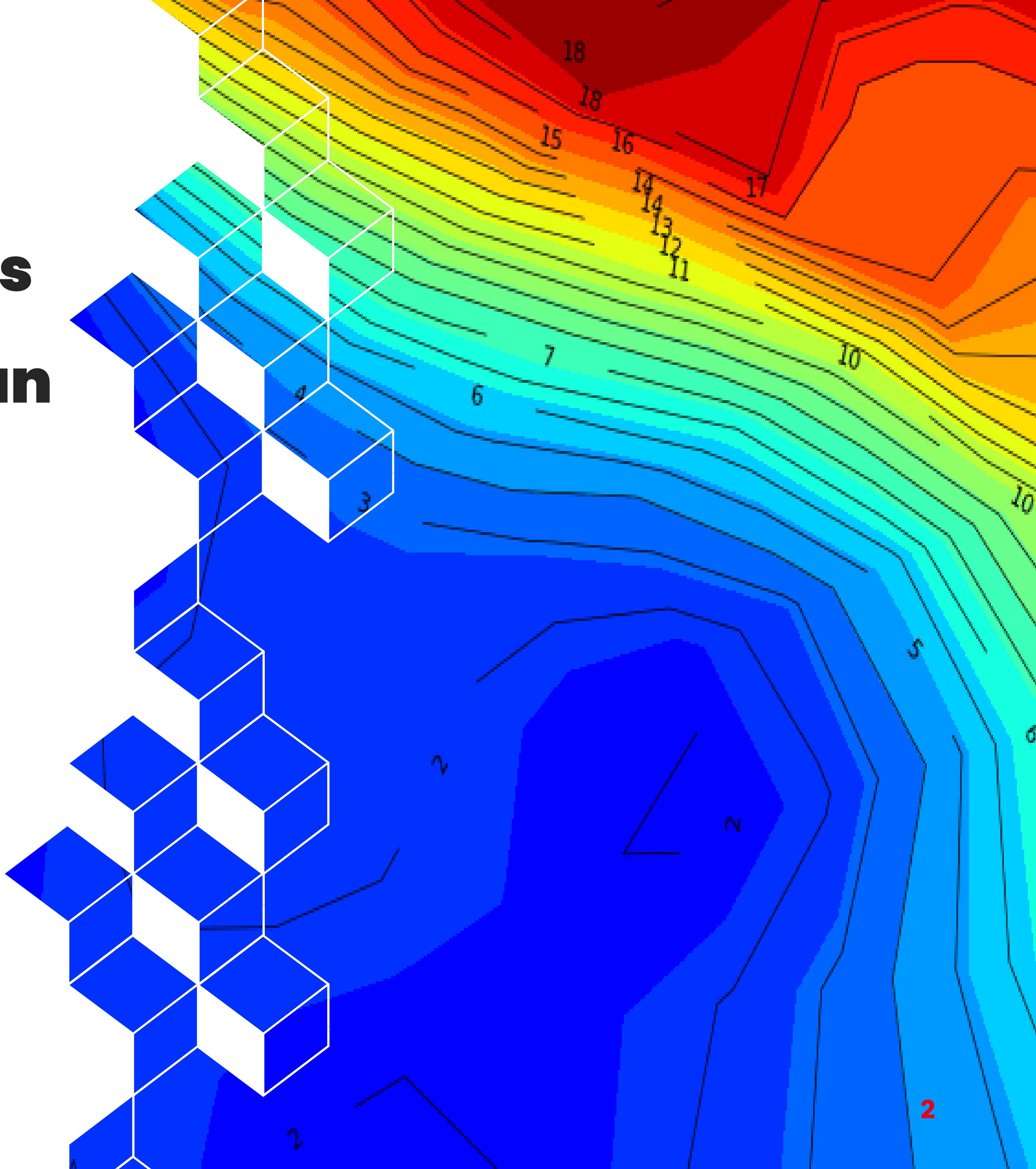
PhD Days - CEA Cadarache – IP2I Lyon

Clémentine Azam

PhD directors:
Dany Davesne *davesne@ipnl.in2p3.fr*
Alessandro Pastore *alessandro.pastore@cea.fr*

Summary

1. **Context and PhD motivations**
2. **Quadrupole Bohr Hamiltonian formalism**
3. **Benchmark with analytical potential**
4. **Microscopic calculations**
5. **Conclusions and perspectives**

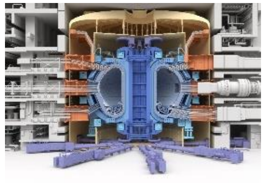


1. Context and PhD motivations

1. Context and PhD motivations

Propulsion navale

Réacteur Jules Horowitz



ITER

Centrale REP

cea

IRESNE

DER

SPRC

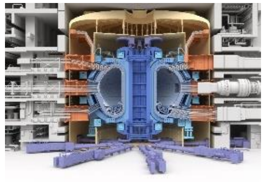
LEPh

Multiphysics simulation code

1. Context and PhD motivations


Propulsion navale


Réacteur Jules Horowitz


ITER


Centrale REP

IRESNE

DER

SPRC

LEPh

Multiphysics simulation code

Nuclear data

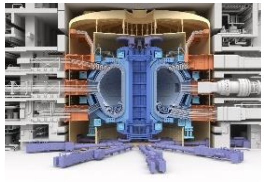
What are nuclear data ?

- Cross sections
- Fission yields
- TKE
- Fragments (A, Z, spin …)
- Distributions
- Reaction products
- …

1. Context and PhD motivations


Propulsion navale


Réacteur Jules Horowitz


ITER


Centrale REP

Multiphysics simulation code ← **Nuclear data** ← ?

What are nuclear data ?

- Cross sections
- Fission yields
- TKE
- Fragments (A, Z, spin …)
- Distributions
- Reaction products
- …

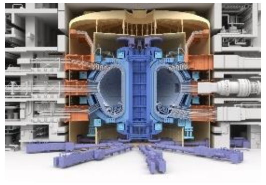
How to obtain these data ?

1. **EXPERIMENTS**

1. Context and PhD motivations


Propulsion navale


Réacteur Jules Horowitz


ITER


Centrale REP

cea
IRESNE
DER
SPRC
LEPh

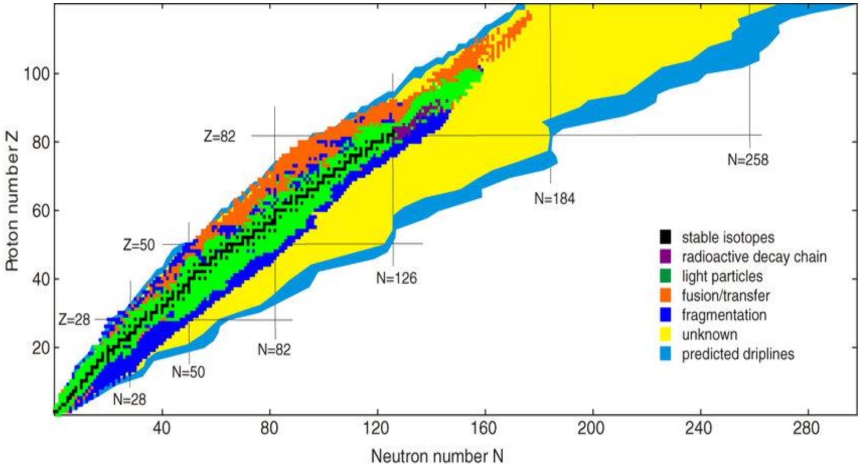
Multiphysics simulation code ← Nuclear data ← ?

What are nuclear data ?

- Cross sections
- Fission yields
- TKE
- Fragments (A, Z, spin …)
- Distributions
- Reaction products
- …

How to obtain these data ?

1. **EXPERIMENTS**
2. **MODELS** (CONRAD, FIFRELIN)



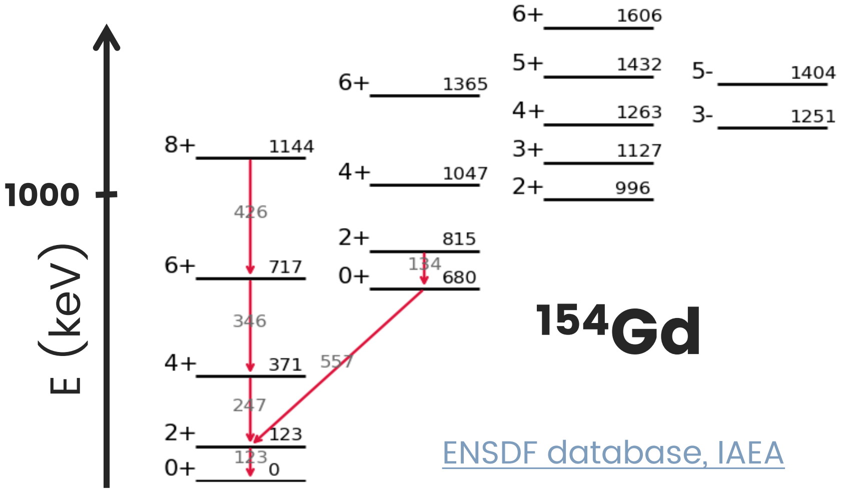
Microscopic data

- Pre-emission neutron fission yields
- Levels densities
- Transition probabilities
- …

➡ **Need a predictive model to explain all nuclear observables along the chart**

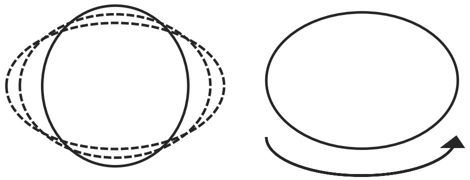
1. Context and PhD motivations

Spectra and transition strengths



ENSDF database, IAEA

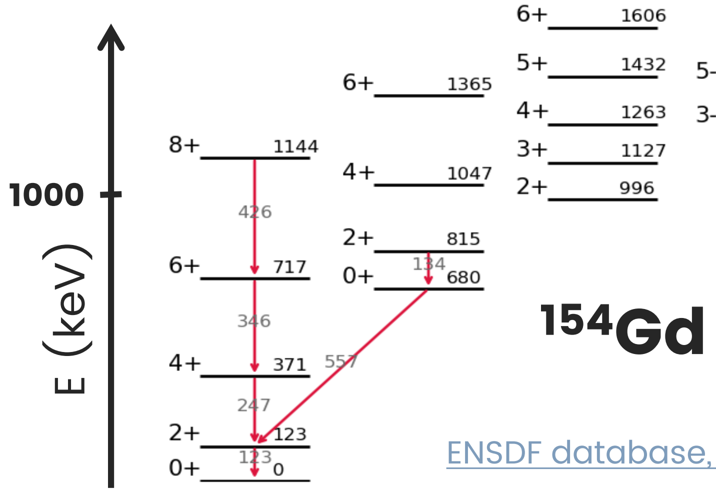
- → Angular momentum
- → Level parities : { + / - }
- → Modes :



Vibrations **Rotations**

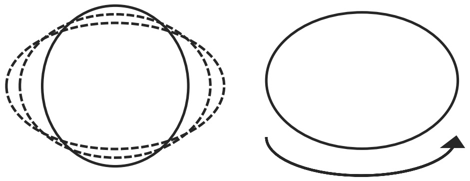
1. Context and PhD motivations

Spectra and transition strengths



ENSDF database, IAEA

- → Angular momentum
- → Level parities : { + / -
- → Modes :



Vibrations **Rotations**

GCM

QRPA

Rigid rotor

...

Bohr Hamiltonian

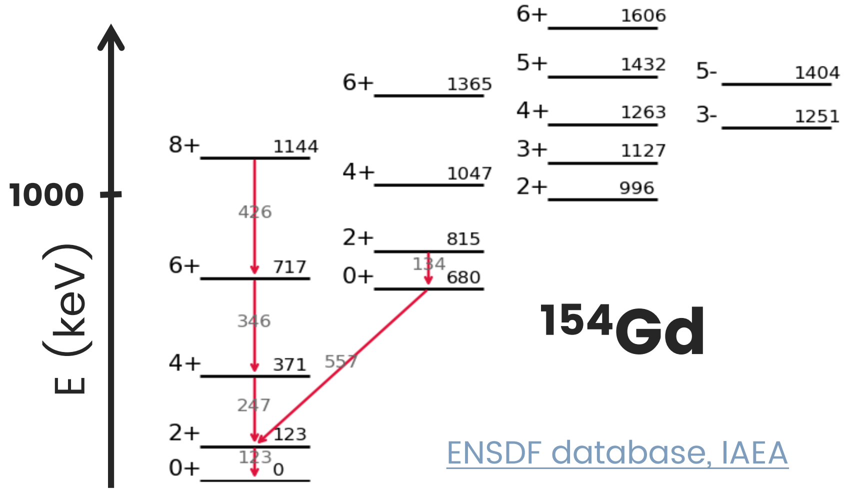
Why choose Quadrupole Bohr Hamiltonian ?

- \+ Vibrational et rotational
- \+ Fast

- \- Even-even nucleus
- \- Positive parity levels

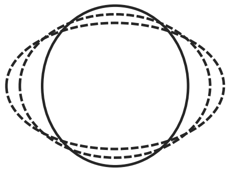
1. Context and PhD motivations

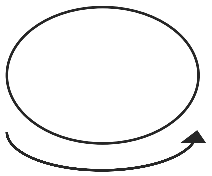
Spectra and transition strengths



ENSDF database, IAEA

- → Angular momentum
- → Level parities : { + / -
- → Modes :





Vibrations **Rotations**

Why choose Quadrupole Bohr Hamiltonian ?

- \+ Vibrational et rotational
- \+ Fast

- \- Even-even nucleus
- \- Positive parity levels ←

PhD objectives ?

- ❑ Quadrupole Bohr Hamiltonian formalism
- ❑ Bohr Hamiltonian code
- ❑ Obtain levels scheme

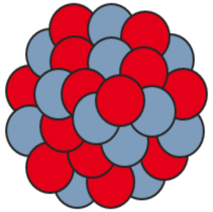
→ Octupole degrees of freedom

A. Dobrowolski, K. Mazurek, and A. Gozdz -2016

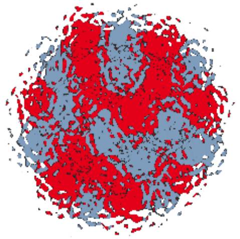
2. Quadrupole Bohr Hamiltonien formalism

2. Quadrupole Bohr Hamiltonien formalism

Step 1 : Definition of collectives parameters



A nucleons



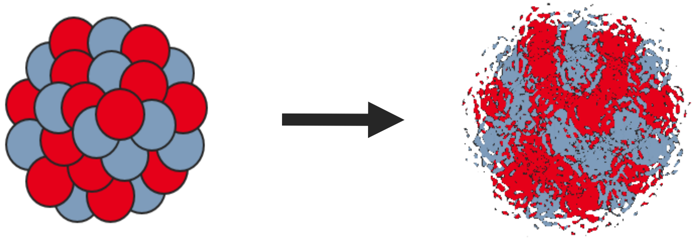
Nuclear surface oscillations

Aage Bohr - 1952

$$R(\theta, \Phi, t) = R_0\left(1 + \sum_{\lambda=0}^{\infty}\sum_{\mu=-\lambda}^{\lambda} \alpha_{\lambda\mu}(t) Y_{\lambda\mu}^{*}(\theta, \Phi)\right)$$

2. Quadrupole Bohr Hamiltonien formalism

Step 1 : Definition of collectives parameters

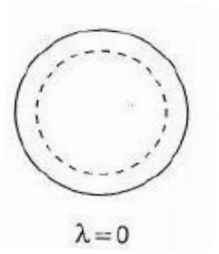


A nucleons

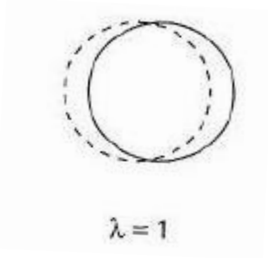
Nuclear surface oscillations

Aage Bohr - 1952

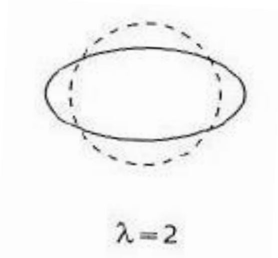
$$R(\theta, \Phi, t) = R_0 \left(1 + \sum_{\lambda=0}^{\infty} \sum_{\mu=-\lambda}^{\lambda} \boxed{\alpha_{\lambda\mu}(t)} Y^*_{\lambda\mu}(\theta, \Phi) \right)$$



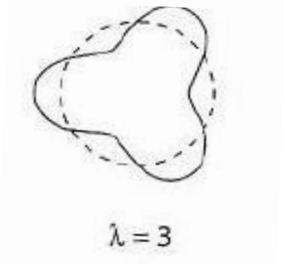
Monopole :
Volume variations



Dipole :
Center of mass



Quadrupole :
Elongation



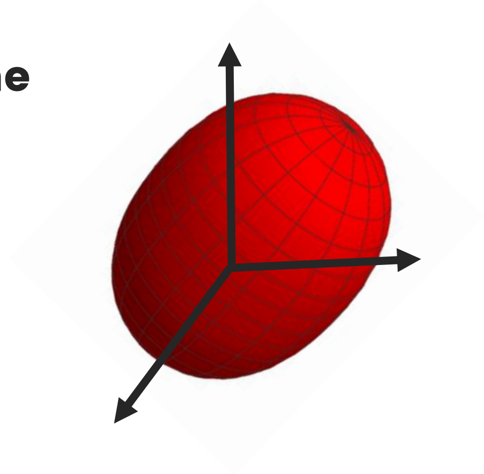
Octupole :
Asymmetric deformation

2. Quadrupole Bohr Hamiltonien formalism

Step 1 : Definition of collectives parameters

Laboratory frame

$$\alpha_2 = \begin{pmatrix} \alpha_{22} \\ \alpha_{21} \\ \alpha_{20} \\ \alpha_{2-1} \\ \alpha_{2-2} \end{pmatrix}$$

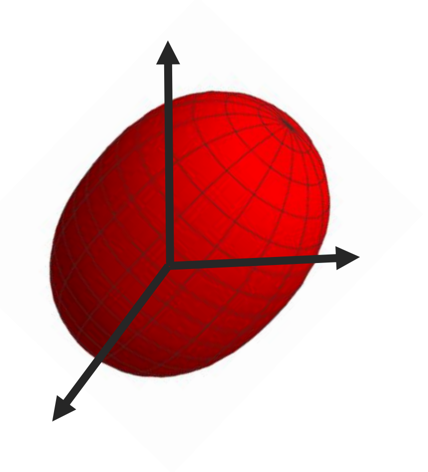


2. Quadrupole Bohr Hamiltonien formalism

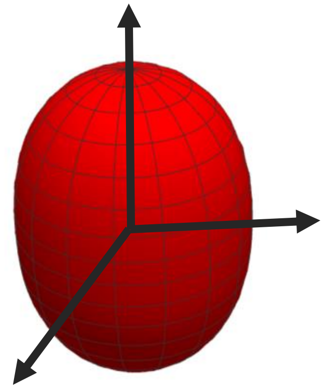
Step 1 : Definition of collectives parameters

Laboratory frame

$$\alpha_2 = \begin{pmatrix} \alpha_{22} \\ \alpha_{21} \\ \alpha_{20} \\ \alpha_{2-1} \\ \alpha_{2-2} \end{pmatrix}$$



Rotation
Euler angles
Ω=(Φ,θ,Ψ)



Intrinsic frame

$$\alpha_2 = \begin{pmatrix} a_2 \\ 0 \\ a_0 \\ 0 \\ a_2 \end{pmatrix} \quad \begin{aligned} a_0 &= \beta\cos\gamma \\ a_2 &= \beta\sin\gamma \end{aligned}$$

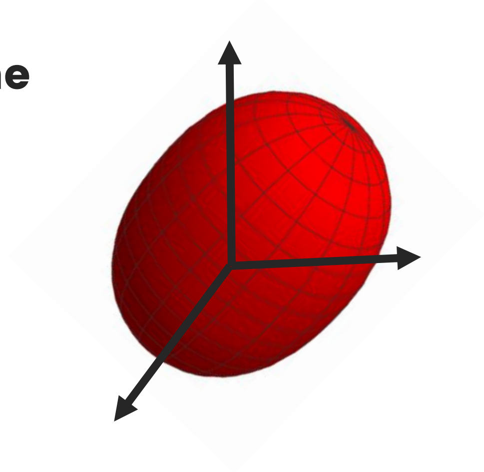
$\{\boldsymbol{\beta},\boldsymbol{\gamma},\boldsymbol{\Phi},\boldsymbol{\theta},\boldsymbol{\Psi}\}$

2. Quadrupole Bohr Hamiltonien formalism

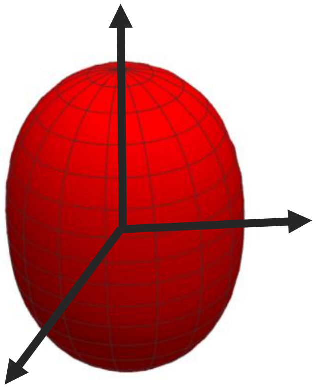
Step 1 : Definition of collectives parameters

Laboratory frame

$$\alpha_2 = \begin{pmatrix} \alpha_{22} \\ \alpha_{21} \\ \alpha_{20} \\ \alpha_{2-1} \\ \alpha_{2-2} \end{pmatrix}$$



Rotation
Euler angles
$\Omega=(\Phi,\theta,\Psi)$

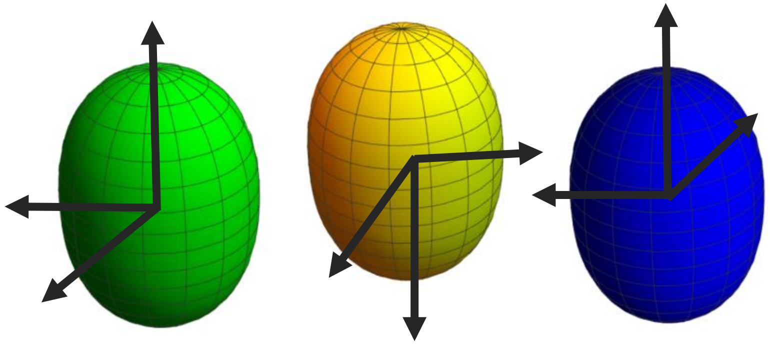


Intrinsic frame

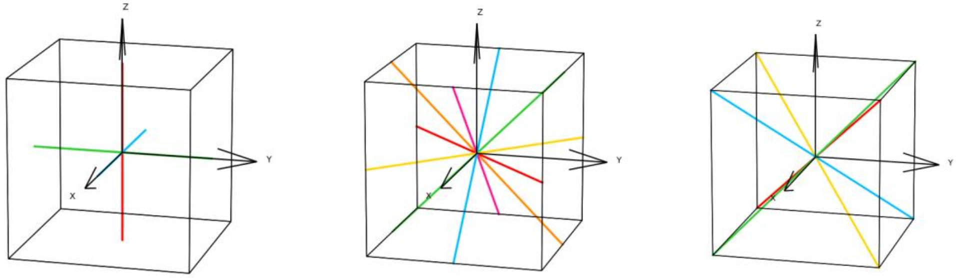
$$\alpha_2 = \begin{pmatrix} a_2 \\ 0 \\ a_0 \\ 0 \\ a_2 \end{pmatrix} \quad \begin{aligned} a_0 &= \beta \cos\gamma \\ a_2 &= \beta \sin\gamma \end{aligned}$$

$\{\boldsymbol{\beta}, \boldsymbol{\gamma}, \boldsymbol{\Phi}, \boldsymbol{\theta}, \boldsymbol{\Psi}\}$

There are 48 ways to position the frame within the intrinsic axes of the nuclei.



= Octahedral group O



2. Quadrupole Bohr Hamiltonien formalism

Step 2 : Obtain collective quantum Hamiltonian

Classical Hamiltonian

$$\hat{H}_{coll} = \frac{1}{2\sqrt{|\det(B_{2,2})|}} \sum_{\mu,\nu} \dot{\alpha}_{2\mu} B^{lab}_{2\mu,2\nu}(\alpha_2)\dot{\alpha}_{2\nu} + V_{coll}(\alpha_2)$$

2. Quadrupole Bohr Hamiltonien formalism

Step 2 : Obtain collective quantum Hamiltonian

Classical Hamiltonian

$$\hat{H}_{coll} = \frac{1}{2\sqrt{|\det(B_{2,2})|}} \sum_{\mu,\nu} \dot{\alpha}_{2\mu} B^{lab}_{2\mu,2\nu}(\alpha_2)\dot{\alpha}_{2\nu} + V_{coll}(\alpha_2)$$

Podolsky-Pauli prescription

$$\hat{H}_{coll} = \frac{1}{2\sqrt{|\det(B_{2,2})|}} \sum_{\mu,\nu} \hat{\pi}_2^{\mu} \sqrt{\det(\boldsymbol{B}_{2,2})}\, G_{2\mu,2\nu}(\alpha_2)\hat{\pi}_2^{\nu} - V_{coll}(\alpha_2)$$

Quantum Hamiltonian

$$\hat{\boldsymbol{H}}_{coll} = \hat{\boldsymbol{H}}_{vib} + \hat{\boldsymbol{H}}_{rot} + V_{coll}$$

$$\hat{\boldsymbol{H}}_{vib} = -\frac{\hbar^2}{2\sqrt{G}} \Big[\frac{1}{\beta^4}\frac{\partial}{\partial\beta}\beta^4\sqrt{G}\frac{\boldsymbol{B}_{\gamma\gamma}}{G_{vib}}\frac{\partial}{\partial\beta} + \frac{1}{\beta^2\sin 3\gamma}\frac{\partial}{\partial\gamma}\sin 3\gamma\sqrt{G}\frac{\boldsymbol{B}_{\beta\beta}}{G_{vib}}\frac{\partial}{\partial\gamma}$$

$$-\frac{1}{\beta^4}\frac{\partial}{\partial\beta}\beta^3\sqrt{G}\frac{\boldsymbol{B}_{\beta\gamma}}{G_{vib}}\frac{\partial}{\partial\gamma} - \frac{1}{\beta\sin 3\gamma}\frac{\partial}{\partial\gamma}\sin 3\gamma\sqrt{G}\frac{\boldsymbol{B}_{\beta\gamma}}{G_{vib}}\frac{\partial}{\partial\beta} \Big]$$

$$\hat{\boldsymbol{H}}_{rot} = \frac{1}{2}\left[\frac{\hat{L}_x^2}{\boldsymbol{J}_x} + \frac{\hat{L}_y^2}{\boldsymbol{J}_y} + \frac{\hat{L}_z^2}{\boldsymbol{J}_z}\right]$$

$$G = |\det(B)| \qquad G_{vib} = \boldsymbol{B}_{\beta\beta}\boldsymbol{B}_{\gamma\gamma} - \boldsymbol{B}_{\beta\gamma}^2$$

2. Quadrupole Bohr Hamiltonien formalism

Step 2 : Obtain collective quantum Hamiltonian

Classical Hamiltonian

$$\hat{H}_{coll} = \frac{1}{2\sqrt{|\det(B_{2,2})|}} \sum_{\mu,\nu} \dot{\alpha}_{2\mu} B^{lab}_{2\mu,2\nu}(\alpha_2)\dot{\alpha}_{2\nu} + V_{coll}(\alpha_2)$$

Podolsky-Pauli prescription

$$\hat{H}_{coll} = \frac{1}{2\sqrt{|\det(B_{2,2})|}} \sum_{\mu,\nu} \hat{\pi}_2^{\mu} \sqrt{\det(\boldsymbol{B_{2,2}})}\, G_{2\mu,2\nu}(\alpha_2)\hat{\pi}_2^{\nu} - \boldsymbol{V_{coll}}(\alpha_2))$$

Quantum Hamiltonian

$$\boldsymbol{\hat{H}_{coll}} = \boldsymbol{\hat{H}_{vib}} + \boldsymbol{\hat{H}_{rot}} + \boldsymbol{V_{coll}}$$

$$\boldsymbol{\hat{H}_{vib}} = -\frac{\hbar^2}{2\sqrt{G}} \left[\frac{1}{\beta^4}\frac{\partial}{\partial\beta}\beta^4\sqrt{G}\frac{\boldsymbol{B_{\gamma\gamma}}}{G_{vib}}\frac{\partial}{\partial\beta} + \frac{1}{\beta^2 \sin 3\gamma}\frac{\partial}{\partial\gamma}\sin 3\gamma\sqrt{G}\frac{\boldsymbol{B_{\beta\beta}}}{G_{vib}}\frac{\partial}{\partial\gamma} - \frac{1}{\beta^4}\frac{\partial}{\partial\beta}\beta^3\sqrt{G}\frac{\boldsymbol{B_{\beta\gamma}}}{G_{vib}}\frac{\partial}{\partial\gamma} - \frac{1}{\beta \sin 3\gamma}\frac{\partial}{\partial\gamma}\sin 3\gamma\sqrt{G}\frac{\boldsymbol{B_{\beta\gamma}}}{G_{vib}}\frac{\partial}{\partial\beta} \right]$$

$$\boldsymbol{\hat{H}_{rot}} = \frac{1}{2}\left[\frac{\hat{L}_x^2}{\boldsymbol{J_x}} + \frac{\hat{L}_y^2}{\boldsymbol{J_y}} + \frac{\hat{L}_z^2}{\boldsymbol{J_z}}\right]$$

$$G = |\det(B)| \qquad G_{vib} = \boldsymbol{B_{\beta\beta}B_{\gamma\gamma}} - \boldsymbol{B_{\beta\gamma}^2}$$

Mass parameters and inertia

Potential

2. Quadrupole Bohr Hamiltonien formalism

Step 2 : Obtain collective quantum Hamiltonian

$$\hat{H}_{coll} = \hat{H}_{vib} + \hat{H}_{rot} + V_{coll}$$

Phenomenological calculations

$B_{\beta\beta}, B_{\beta\gamma}, B_{\gamma\gamma}, J_x, J_y, J_z$: Constant free parameters to be adjusted

V_{coll} : Phenomenological potential

$\psi(\beta, \gamma, \Phi, \theta, \varphi)$: Analytical solutions

2. Quadrupole Bohr Hamiltonien formalism

Step 2 : Obtain collective quantum Hamiltonian

$$\hat{H}_{coll} = \hat{H}_{vib} + \hat{H}_{rot} + V_{coll}$$

Phenomenological calculations

$B_{\beta\beta}, B_{\beta\gamma}, B_{\gamma\gamma}, J_x, J_y, J_z$: Constant free parameters to be adjusted

V_{coll} : Phenomenological potential

$\psi(\beta,\gamma,\Phi,\theta,\varphi)$: Analytical solutions

Microscopic calculations

$B_{\beta\beta}, B_{\beta\gamma}, B_{\gamma\gamma}, J_x, J_y, J_z, V_{coll}$ Microscopic calculations for each deformation (β,γ)

$\Psi(\beta,\gamma,\Phi,\theta,\varphi)$ Construction of the wave function basis J. Libert, P. Quentin - 1982

$< \Psi|\hat{H}_{coll}|\Psi >$ Diagonalization

2. Quadrupole Bohr Hamiltonien formalism

Step 3 : Construction of function basis

J. Libert, P. Quentin – 1982

$$\Psi^{IM}_{Lmn}(\beta,\gamma,\Phi,\theta,\Psi) = e^{-\mu\beta^2/2}\beta^n \begin{Bmatrix}\cos m\gamma \\ \sin m\gamma\end{Bmatrix} D^{I*}_{ML}(\Phi,\theta,\Psi)$$

$$-I \leq L \leq I$$
$$m = 0\,,1\ \ldots, m_{max}$$
$$n = m, m+2, \ldots$$

→ All these functions constitute a representation of the continuous group of rotations in space $SO(3)$

2. Quadrupole Bohr Hamiltonien formalism

Step 3 : Construction of function basis

J. Libert, P. Quentin – 1982

$$\Psi^{IM}_{Lmn}(\beta,\gamma,\Phi,\theta,\Psi) = e^{-\mu\beta^2/2}\beta^n \begin{Bmatrix}\cos m\gamma \\ \sin m\gamma\end{Bmatrix} D^{I*}_{ML}(\Phi,\theta,\Psi)$$

$$-I \leq L \leq I$$
$$m = 0\,,1\ \ldots, m_{max}$$
$$n = m, m+2, \ldots$$

→ All these functions constitute a representation of the continuous group of rotations in space $SO(3)$

2. Quadrupole Bohr Hamiltonien formalism

Step 3 : Construction of function basis

J. Libert, P. Quentin – 1982

$$\Psi^{IM}_{Lmn}(\beta,\gamma,\Phi,\theta,\Psi) = e^{-\mu\beta^2/2}\beta^n \begin{Bmatrix}\cos m\gamma \\ \sin m\gamma\end{Bmatrix} D^{I*}_{ML}(\Phi,\theta,\Psi)$$

$-I \leq L \leq I$

$m = 0\,,1\ \ldots, m_{max}$

$n = m, m+2, \ldots$

→ All these functions constitute a representation of the continuous group of rotations in space $SO(3)$

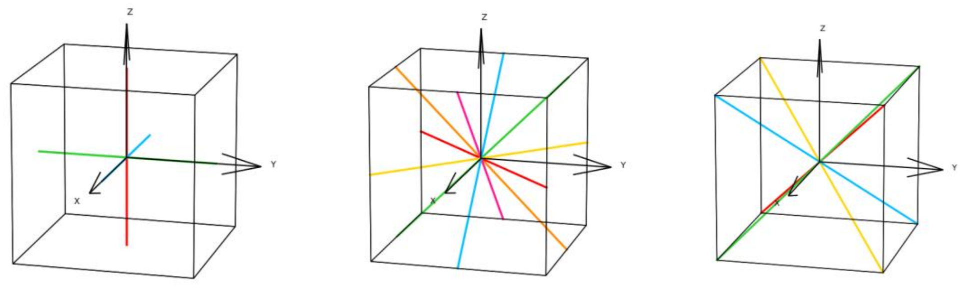
1 Symmetries of the problem

Laboratory frame — **Rotation** → **Intrinsic frame**

48 ways to define the inrtinsic frame

↓

Wave funtions must be invariants



= Octahedral group O_h

→ **R_1 R_2 R_3**

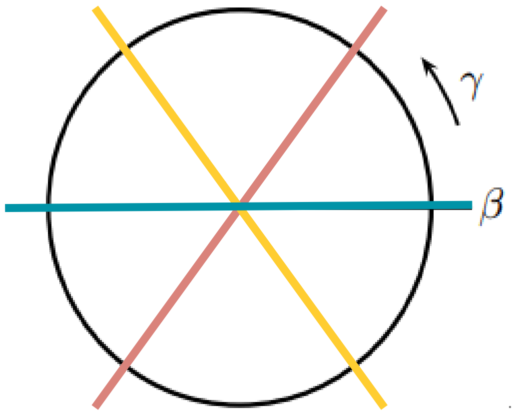
$$R_k \Psi^{IM}_{Lmn} = \Psi^{IM}_{Lmn}$$

2. Quadrupole Bohr Hamiltonien formalism

Step 3 : Construction of function basis

2 Definition of the matrix elements of the Hamiltonian $< \Psi|\hat{H}_{coll}\,|\Psi >$

Problem ?



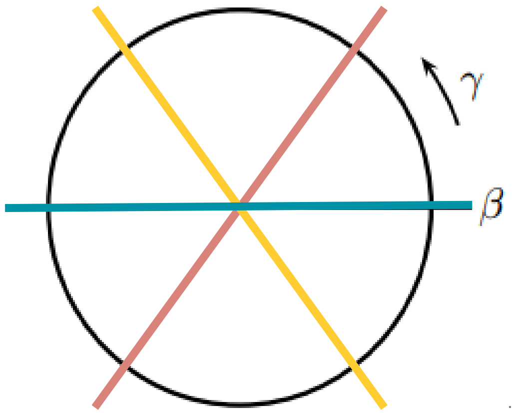
$$\hat{H}_{rot} = \frac{1}{2}\left[\frac{\hat{L}_x^2}{J_x} + \frac{\hat{L}_y^2}{J_y} + \frac{\hat{L}_z^2}{J_z}\right]$$

2. Quadrupole Bohr Hamiltonien formalism

Step 3 : Construction of function basis

2 Definition of the matrix elements of the Hamiltonian $< \Psi | \hat{H}_{coll} | \Psi >$

Problem ?



$$\hat{H}_{rot} = \frac{1}{2}\left[\frac{\hat{L}_x^2}{J_x} + \frac{\hat{L}_y^2}{J_y} + \frac{\hat{L}_z^2}{J_z}\right]$$

Solution ? After the symmetrization procedure, our **basis is redundant**

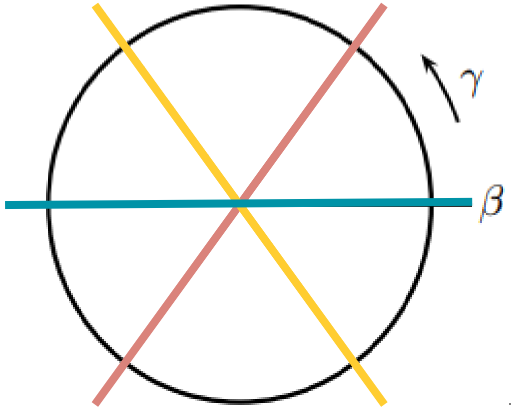
Making **linear combinations** → $|\Psi> = |\Psi> = |\Psi> = 0$

2. Quadrupole Bohr Hamiltonien formalism

Step 3 : Construction of function basis

2 Definition of the matrix elements of the Hamiltonian $< \Psi|\hat{H}_{coll}\,|\Psi >$

Problem ?



$$\hat{H}_{rot} = \frac{1}{2}\left[\frac{\hat{L}_x^2}{J_x} + \frac{\hat{L}_y^2}{J_y} + \frac{\hat{L}_z^2}{J_z}\right]$$

Solution ? After the symmetrization procedure, our **basis is redundant**

Making **linear combinations** → $|\Psi > = |\Psi >= |\Psi >= 0$

How many linearly independent functions?

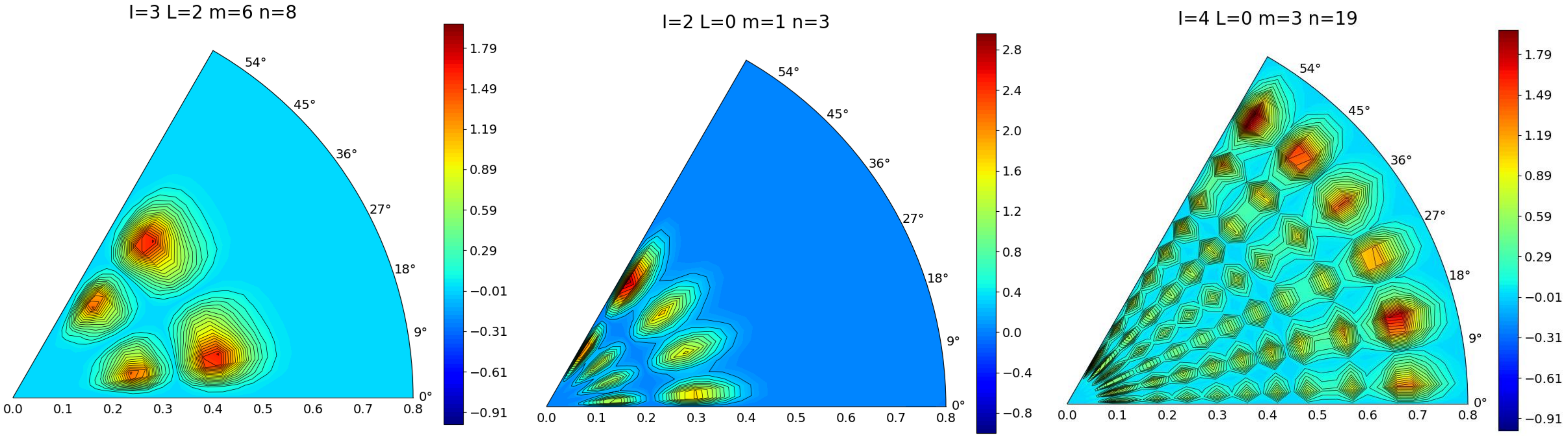
→ I want to know the number of linearly independent functions that can be formed from this set of functions, taking into account the symmetries of the O_h group

→ This is equivalent to **decomposing the problem into the irreducible representations of the O_h symmetry group**

2. Quadrupole Bohr Hamiltonien formalism

Step 3 : Construction of function basis

3 **Orthogonalization** $\int d\beta \int d\gamma \int d\Omega \sqrt{G}\, \beta^4 |\sin 3\gamma|\, \Psi^{I'M'}_{L'm'n'}\, \Psi^{IM}_{Lmn} = \delta_{II'}\delta_{MM'}\delta_{LL'}\delta_{mm'}\delta_{nn'}$

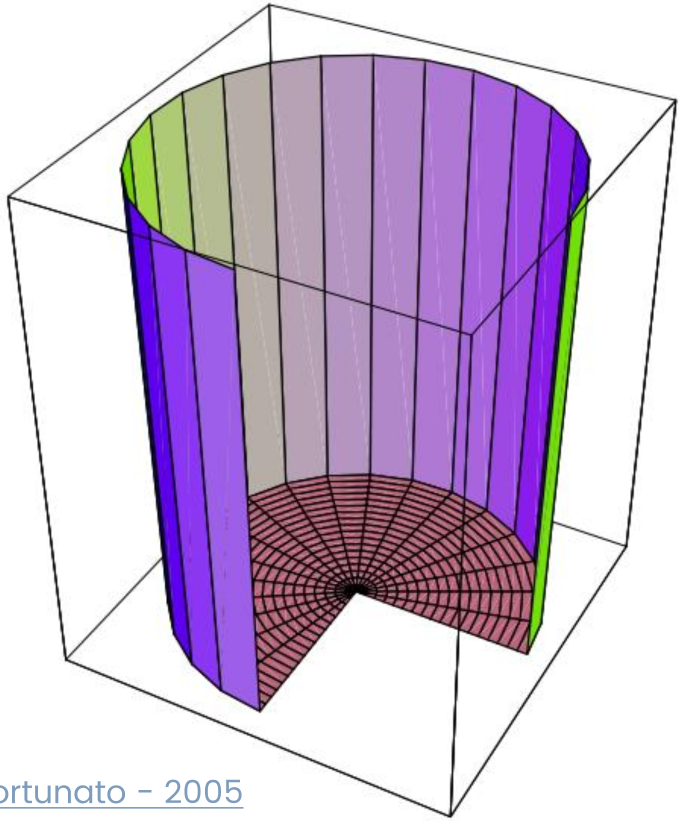


Probability density (on the βγ-plane) is obtained by integration of |Ψ|² over the Euler angles $P = \sum_K \sqrt{G}\beta^4 |\sin 3\gamma|\, \left|\Psi^{IM}_{Lmn}(\beta,\gamma)\right|^2$

3. Benchmark with analytical potential

Benchmark with analytical potential

Infinite-square potential



L. Fortunato - 2005

$B = B_{\beta\beta} = B_{\gamma\gamma} = J_x = J_y = J_z = 0.5$
$B_{\beta\gamma} = 0$

$$\Psi(\beta,\gamma,\Omega) = f(\beta)\Phi(\gamma,\Omega)$$

$$\left\{\frac{\hbar^2}{2B}\left(-\frac{1}{\beta^4}\frac{\partial}{\partial\beta}\beta^4\frac{\partial}{\partial\beta}+\frac{\Lambda^2}{\beta^2}\right)+V(\beta)\right\}f(\beta) = Ef(\beta)$$

$$\left\{-\frac{1}{\sin 3\gamma}\frac{\partial}{\partial\gamma}\sin 3\gamma\frac{\partial}{\partial\gamma}+\frac{1}{4}\sum_{k=1}^{3}\frac{\hat{L}_k^2}{\left(\hbar\sin(\gamma-\frac{2\pi}{3}k)\right)^2}\right\}\Phi(\gamma,\Omega) = \Lambda^2\Phi(\gamma,\Omega)$$

➡ Analytical solutions

Studies on basis

$$\Psi^{IM}_{Lmn}(\beta,\gamma,\Phi,\theta,\Psi) = B_{mn}(\beta)\,\Gamma^{I}_{Lmn}(\gamma)\,D^{I*}_{ML}(\Phi,\theta,\Psi)$$

$$-I \leq L \leq I$$
$$m = 0\,,1\ \ldots, m_{max}$$
$$n = m, m+2, \ldots, n_{max}$$

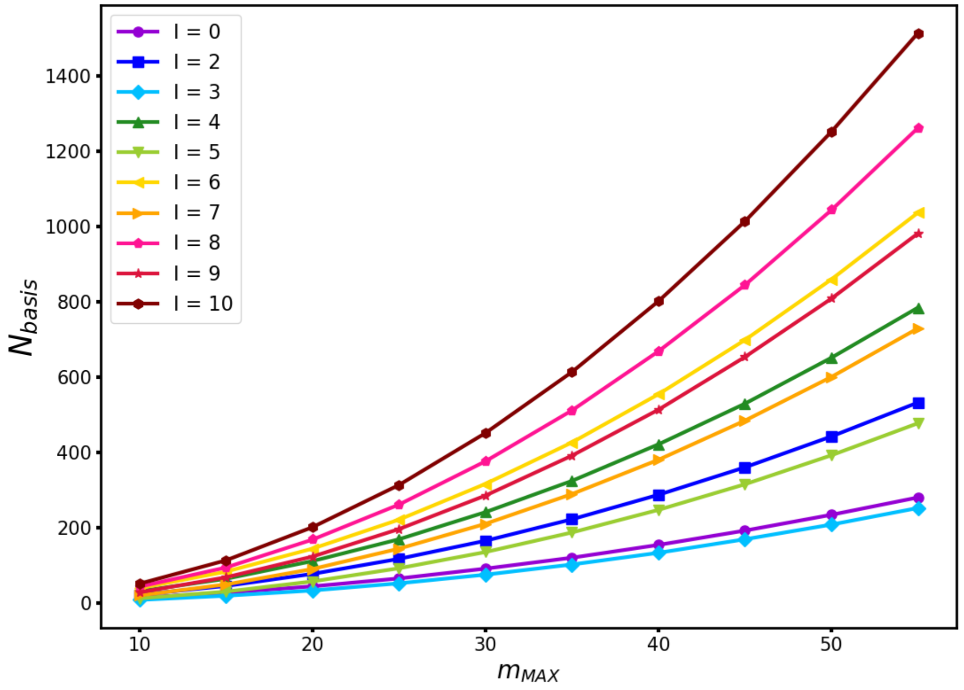
Studies on basis

$$\Psi^{\mathrm{IM}}_{\mathrm{Lmn}}(\beta,\gamma,\Phi,\theta,\Psi) = B_{mn}(\beta)\,\Gamma^{I}_{Lmn}(\gamma)\,\mathrm{D}^{\mathrm{I}*}_{\mathrm{ML}}(\Phi,\theta,\Psi)$$

$$-I \leq L \leq I$$
$$m = 0\,,1\ \ldots, m_{max}$$
$$n = m, m+2, \ldots, n_{max}$$

- $m_{max} \rightarrow$ truncation of the basis

Number of state in function of I and m_{max}



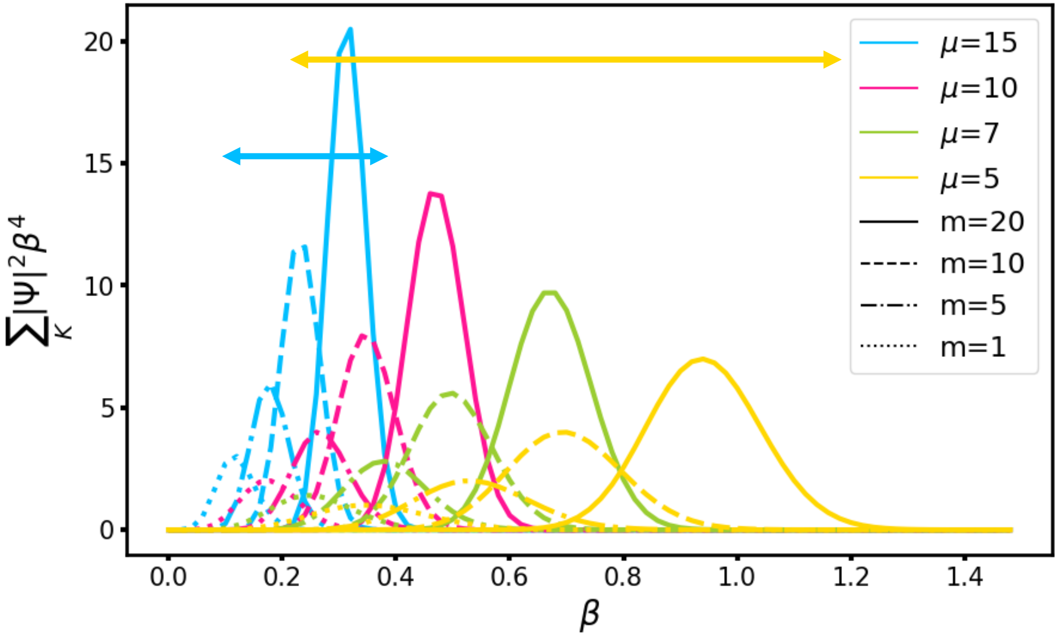
Studies on basis

$$\Psi^{IM}_{Lmn}(\beta,\gamma,\Phi,\theta,\Psi) = B_{mn}(\beta)\,\Gamma^{I}_{Lmn}(\gamma)\,D^{I*}_{ML}(\Phi,\theta,\Psi) \qquad \begin{array}{l} -I \le L \le I \\ m = 0, 1 \,\ldots, m_{max} \\ n = m, m+2, \ldots, n_{max} \end{array}$$

$$e^{-\mu\beta^2/2}$$

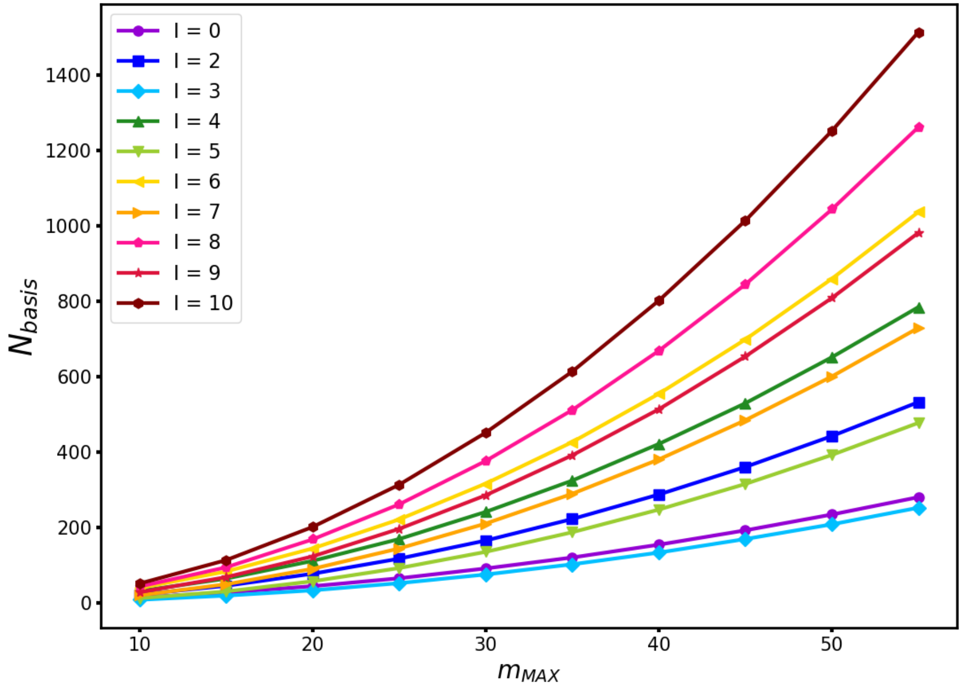
- μ → free parameter

Representation of the basis functions for different values of μ

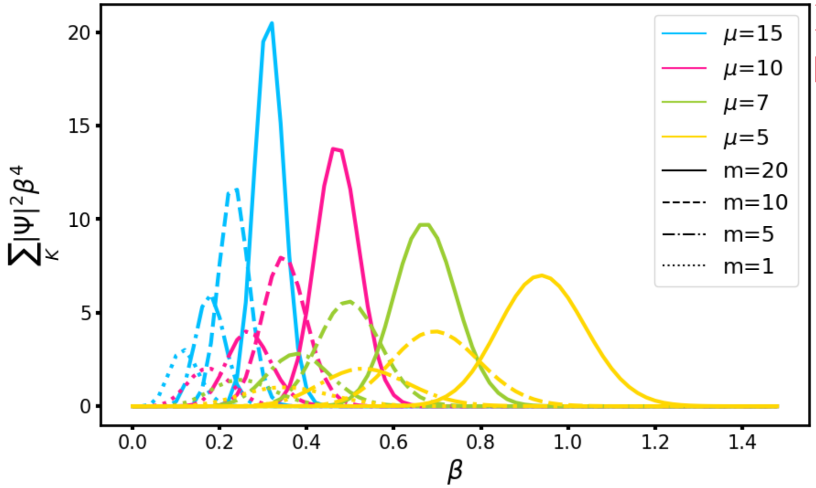


- m_{max} → truncation of the basis

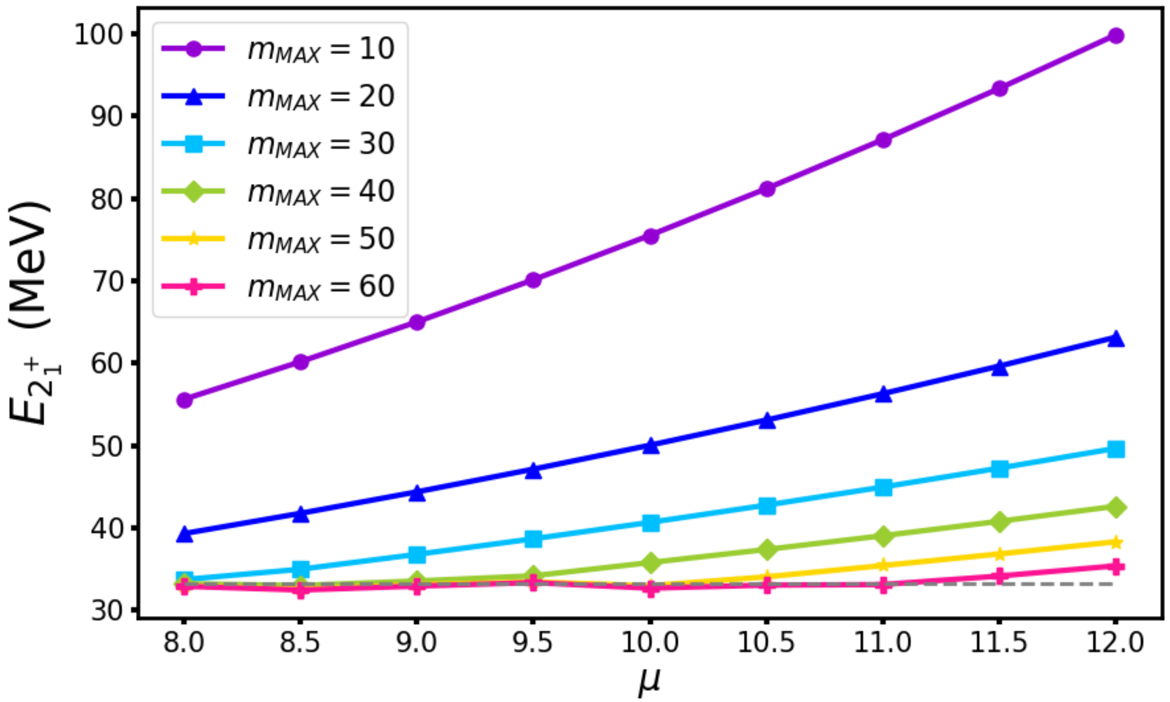
Number of state in function of I and m_{max}



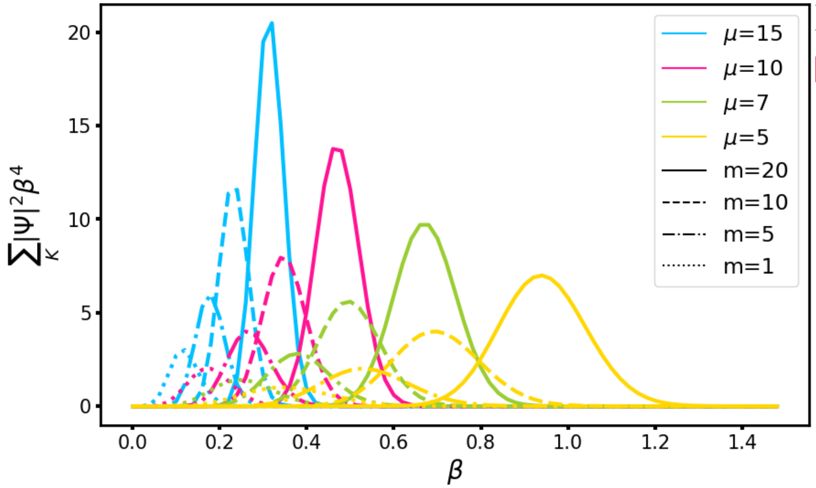
Studies on basis



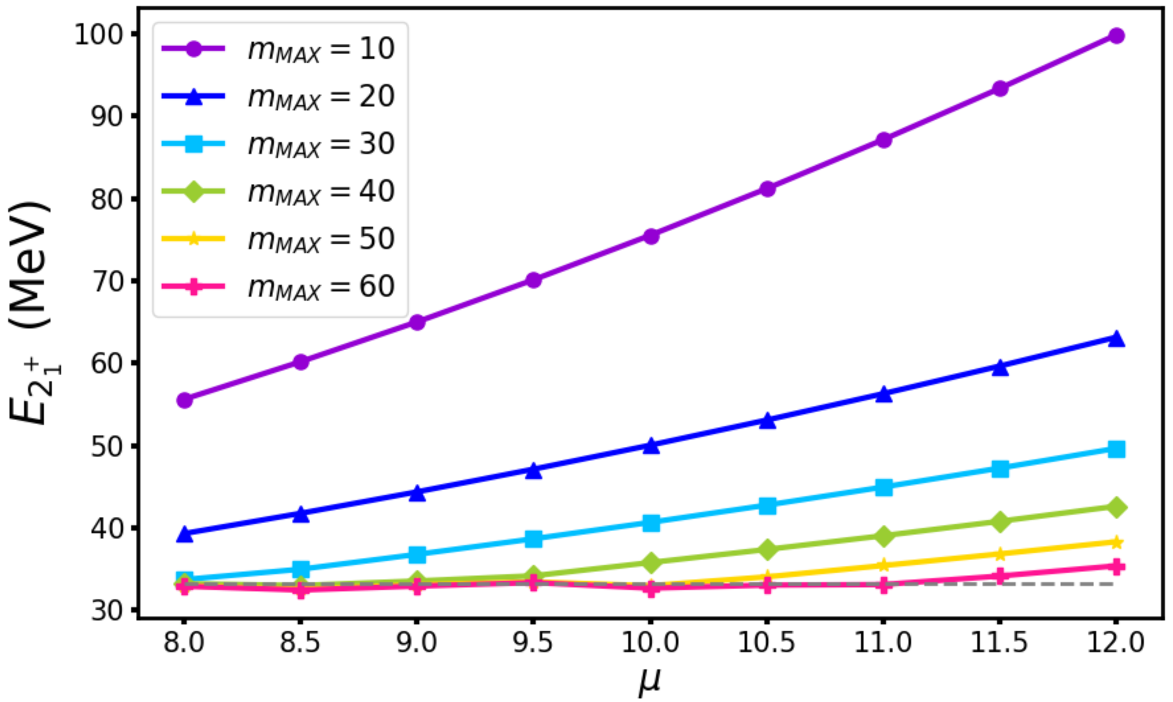
- The larger m_{max}, the more basis functions we have and the less important the value of μ becomes, but the computation time increases
- As the value of μ increases, the basis functions become more localised, leading to a less accurate description of the physical problem.

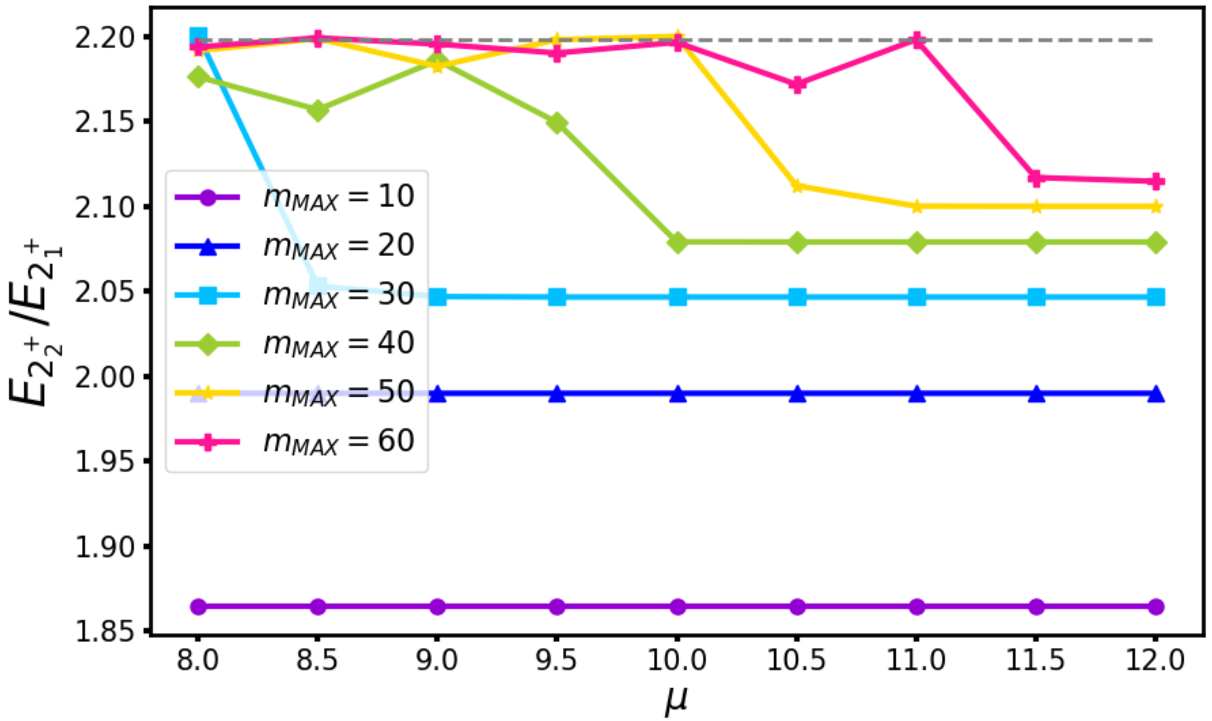


Studies on basis



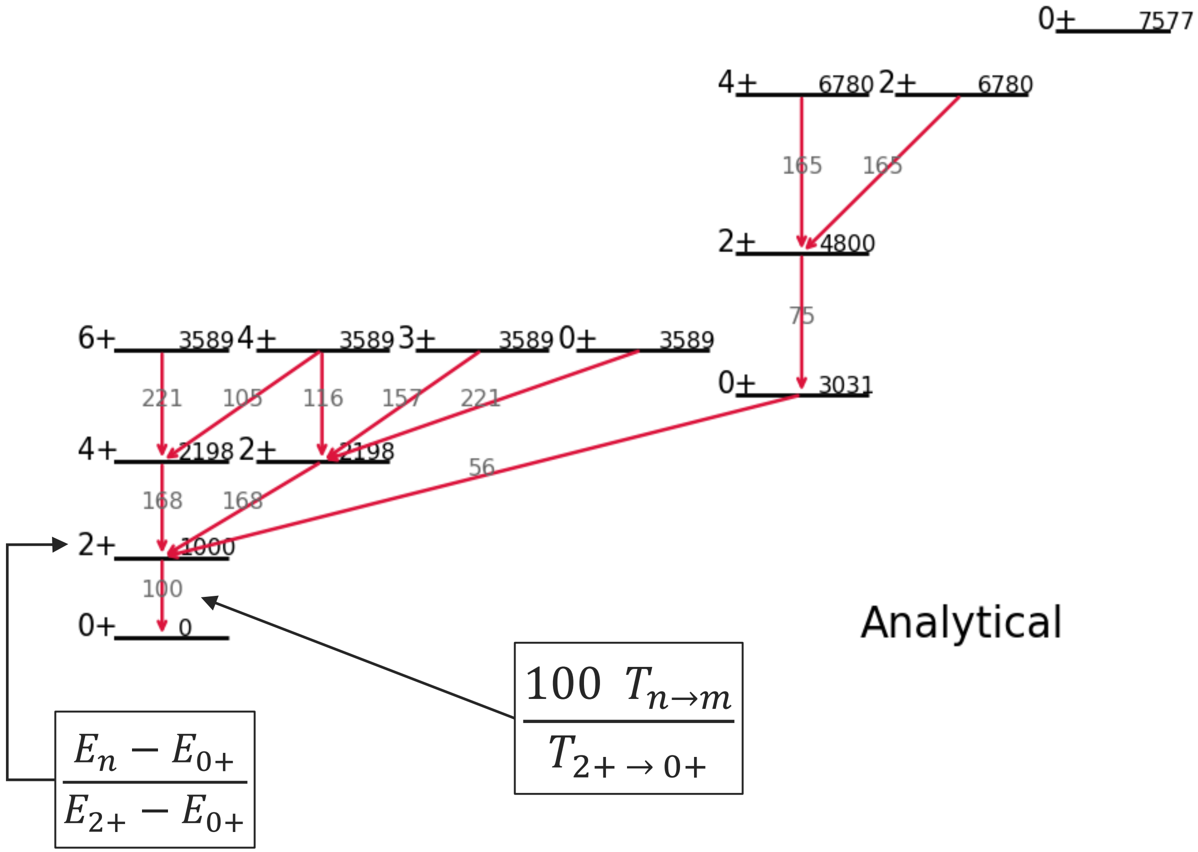
- The larger m_{max}, the more basis functions we have and the less important the value of μ becomes, but the computation time increases
- As the value of μ increases, the basis functions become more localised, leading to a less accurate description of the physical problem.



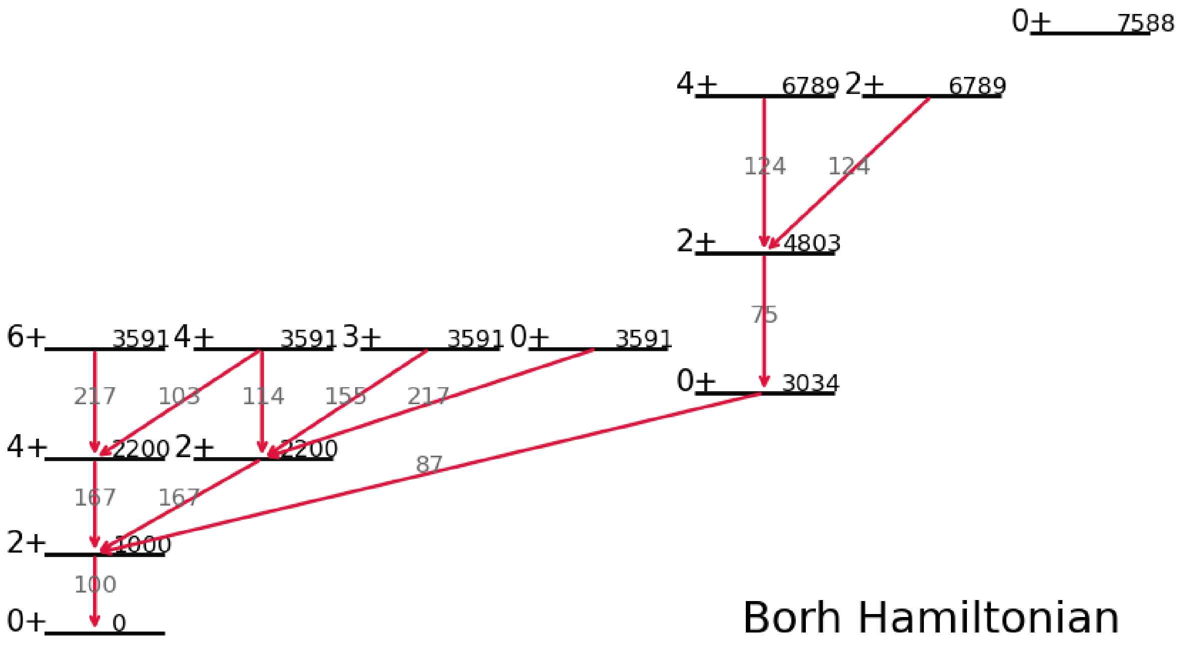


Benchmark with analytical potential

Analytical solutions :



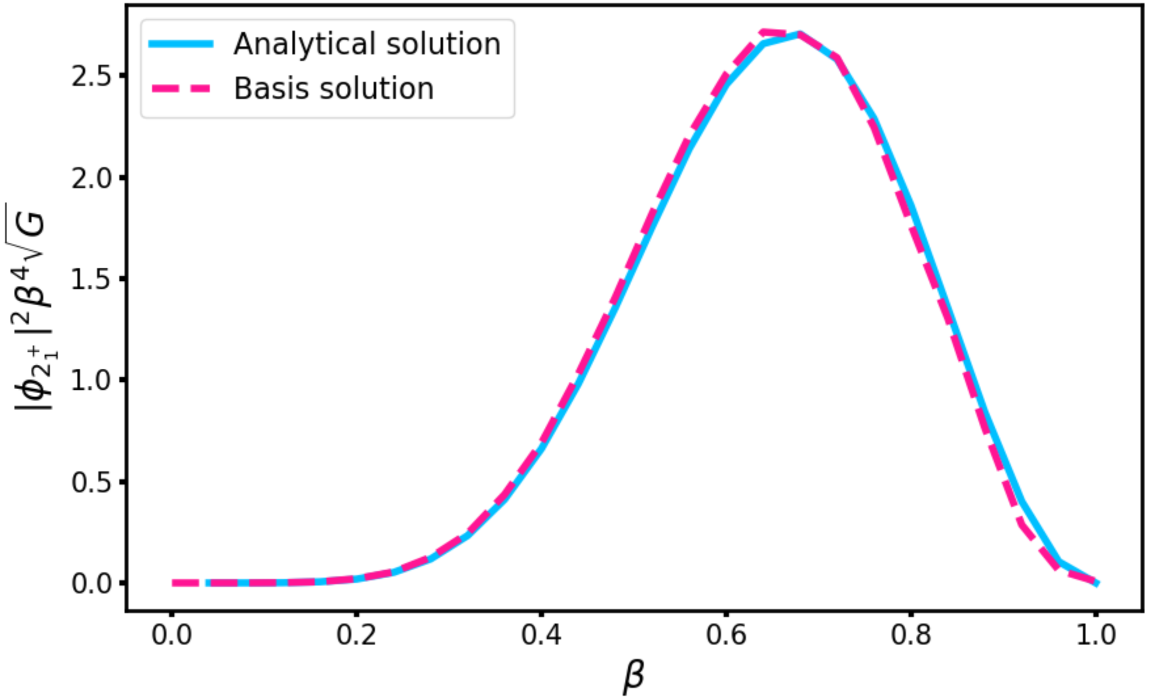
Code results :

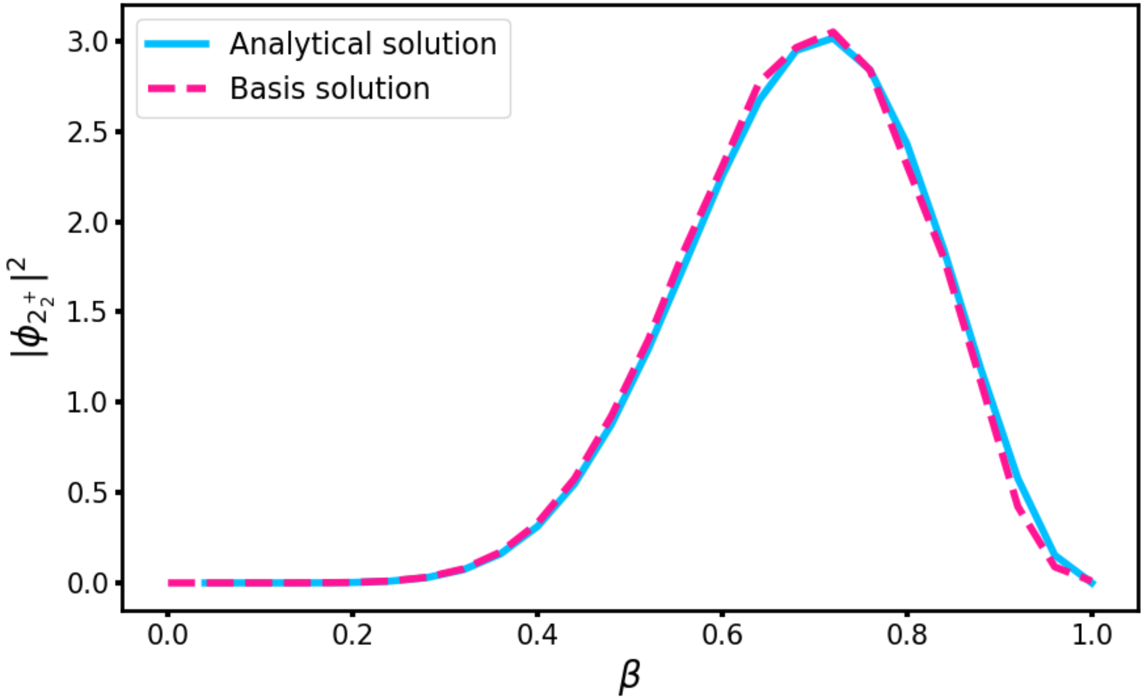


Phenomenological potential + constant mass parameters

Benchmark with analytical potential

Final wave functions for the first two 2^+ states





4. Microscopic calculations

Microscopic input data

Hamiltonien quantique

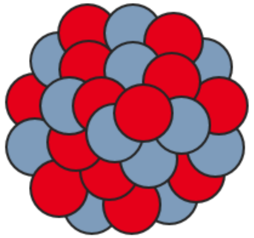
$$\hat{H}_{coll} = \hat{H}_{vib} + \hat{H}_{rot} + V_{coll}$$

$$\hat{H}_{vib} = -\frac{\hbar^2}{2\sqrt{G}}\Big[\frac{1}{\beta^4}\frac{\partial}{\partial\beta}\beta^4\sqrt{G}\frac{B_{\gamma\gamma}}{G_{vib}}\frac{\partial}{\partial\beta} + \frac{1}{\beta^2\sin 3\gamma}\frac{\partial}{\partial\gamma}\sin 3\gamma\sqrt{G}\frac{B_{\beta\beta}}{G_{vib}}\frac{\partial}{\partial\gamma}$$
$$-\frac{1}{\beta^4}\frac{\partial}{\partial\beta}\beta^3\sqrt{G}\frac{B_{\beta\gamma}}{G_{vib}}\frac{\partial}{\partial\gamma} - \frac{1}{\beta\sin 3\gamma}\frac{\partial}{\partial\gamma}\sin 3\gamma\sqrt{G}\frac{B_{\beta\gamma}}{G_{vib}}\frac{\partial}{\partial\beta}\Big]$$

$$\hat{H}_{rot} = \frac{1}{2}\left[\frac{\hat{L}_x^2}{J_x} + \frac{\hat{L}_y^2}{J_y} + \frac{\hat{L}_z^2}{J_z}\right] \qquad G = |\det(B)| \qquad G_{vib} = B_{\beta\beta}B_{\gamma\gamma} - B_{\beta\gamma}^2$$

Microscopic calculations

A-body problem :



Z protons
N neutrons

A quantum system of A interacting particles

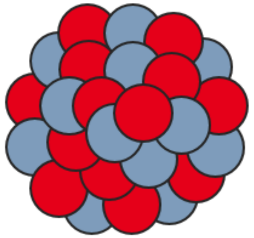
$$\hat{H}|\Psi\rangle = E|\Psi\rangle$$

$$\hat{H} = \sum_{i-1}^{A} \frac{\vec{p_i}^2}{2M} + \frac{1}{2}\sum_{i\neq j=1}^{A} \hat{v}_{ij} + \frac{1}{3!}\sum_{i\neq j\neq k} \hat{v}_{ijk} + \cdots$$

Microscopic calculations

A-body problem :

$$\hat{H}|\Psi\rangle = E|\Psi\rangle$$

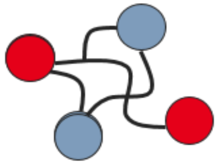


Z protons
N neutrons

A quantum system of A interacting particles

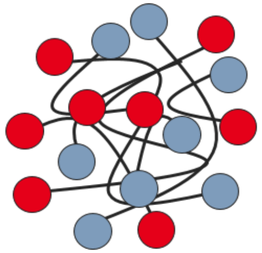
$$\hat{H} = \sum_{i-1}^{A} \frac{\vec{p_i}^2}{2M} + \frac{1}{2}\sum_{i\neq j=1}^{A} \hat{v}_{ij} + \frac{1}{3!}\sum_{i\neq j\neq k} \hat{v}_{ijk} + \cdots$$

Problem n°1: Nuclear interaction $\hat{V}$



QCD (quark + gluons)

Problem n°2: A-body

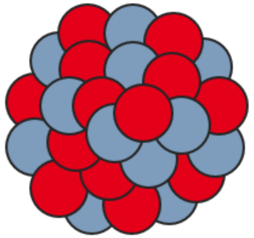


Interaction potential arising from the nucleons themselves

Microscopic calculations

A-body problem :

$$\hat{H}|\Psi\rangle = E|\Psi\rangle$$

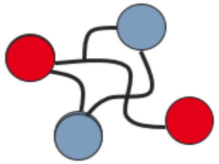


Z protons
N neutrons

A quantum system of A interacting particles

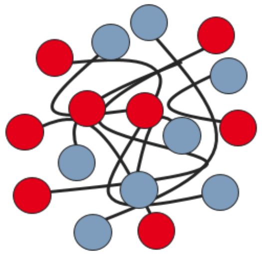
$$\hat{H} = \sum_{i-1}^{A} \frac{\vec{p_i}^2}{2M} + \frac{1}{2}\sum_{i\neq j=1}^{A} \hat{v}_{ij} + \frac{1}{3!}\sum_{i\neq j\neq k} \hat{v}_{ijk} + \cdots$$

Problem n°1: Nuclear interaction $\hat{V}$

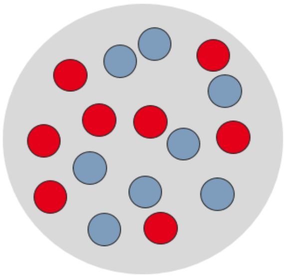


QCD (quark + gluons)

Problem n°2: A-body



Interaction potential arising from the nucleons themselves



\+

Effective interactions

$$\hat{V}_{ij} \approx \hat{V}_{eff}$$

(Skyrme, Gogny …)

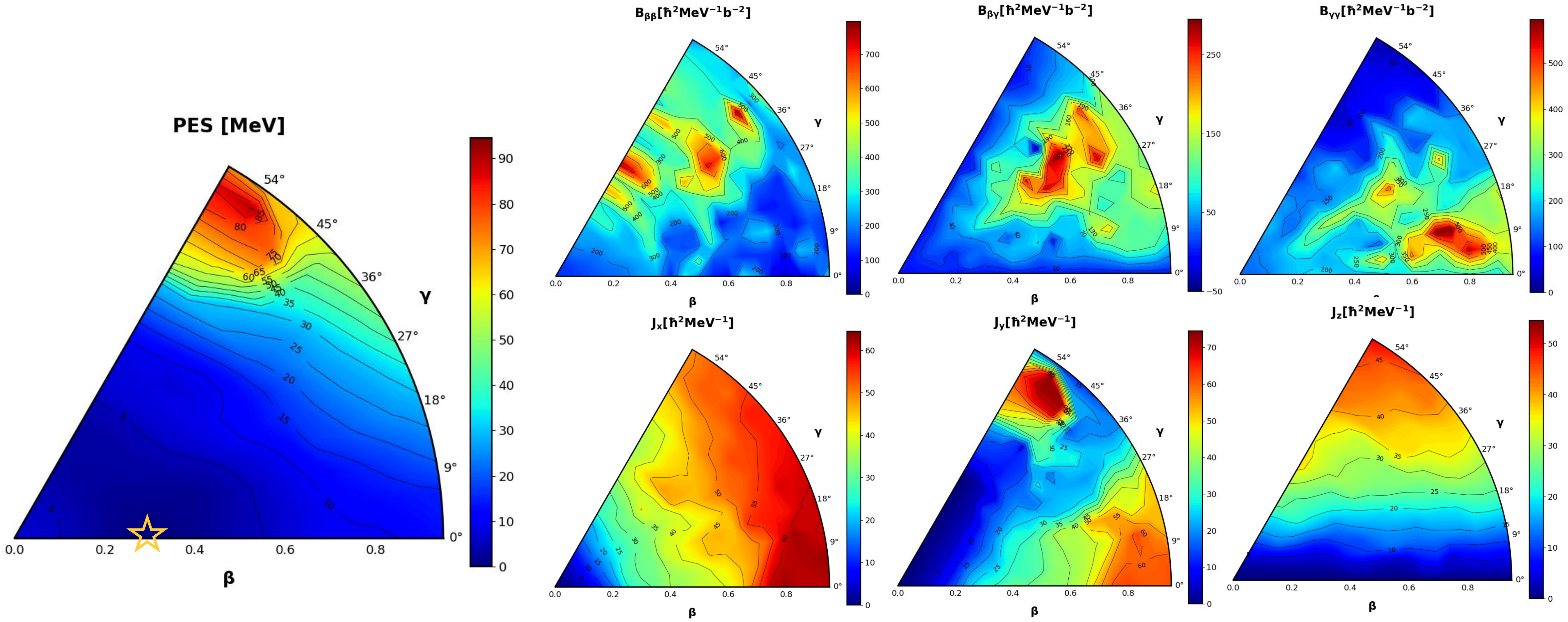
Mean-field methods

Nucleons evolve within the nucleus under the influence of a common potential, which is generated collectively by all of them.

$$\hat{H} = \hat{H}_0 + V_{res}$$

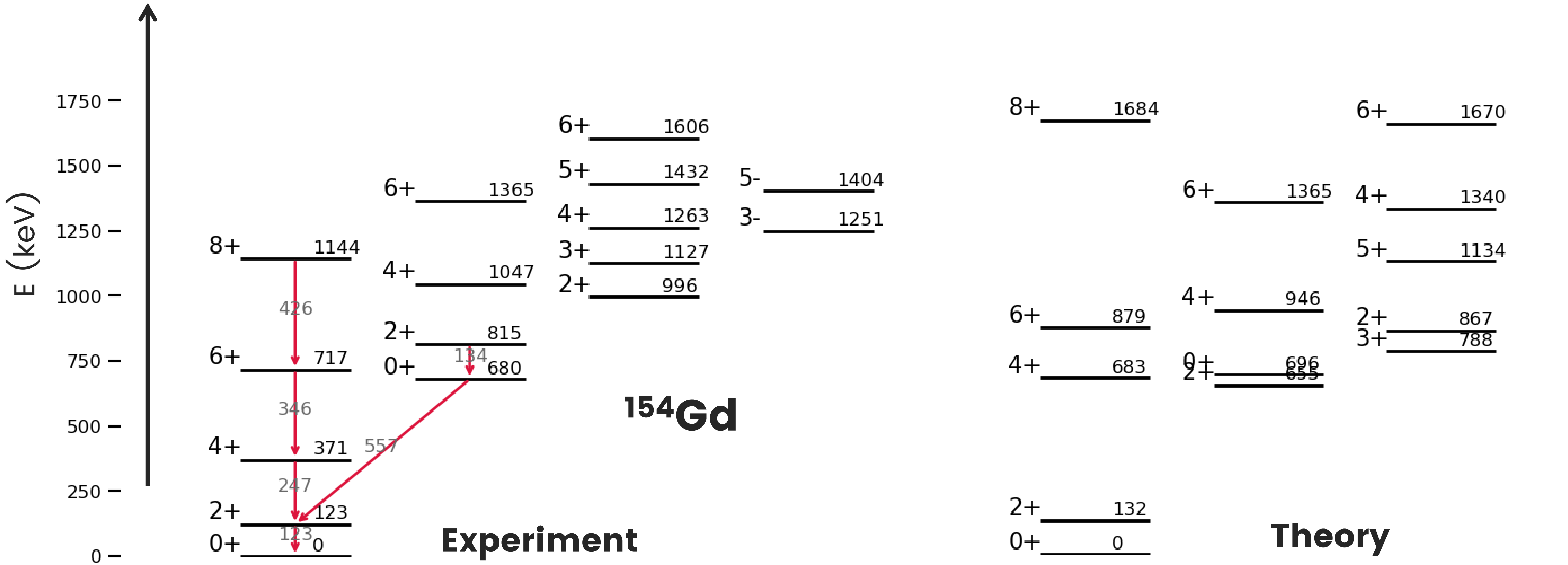
Residual interations:
- Pairing (HFB)
- …

Microscopic data



Result of a PANACEA constrained HFB calculation for ^{154}Gd with D1S

^{154}Gd spectrum

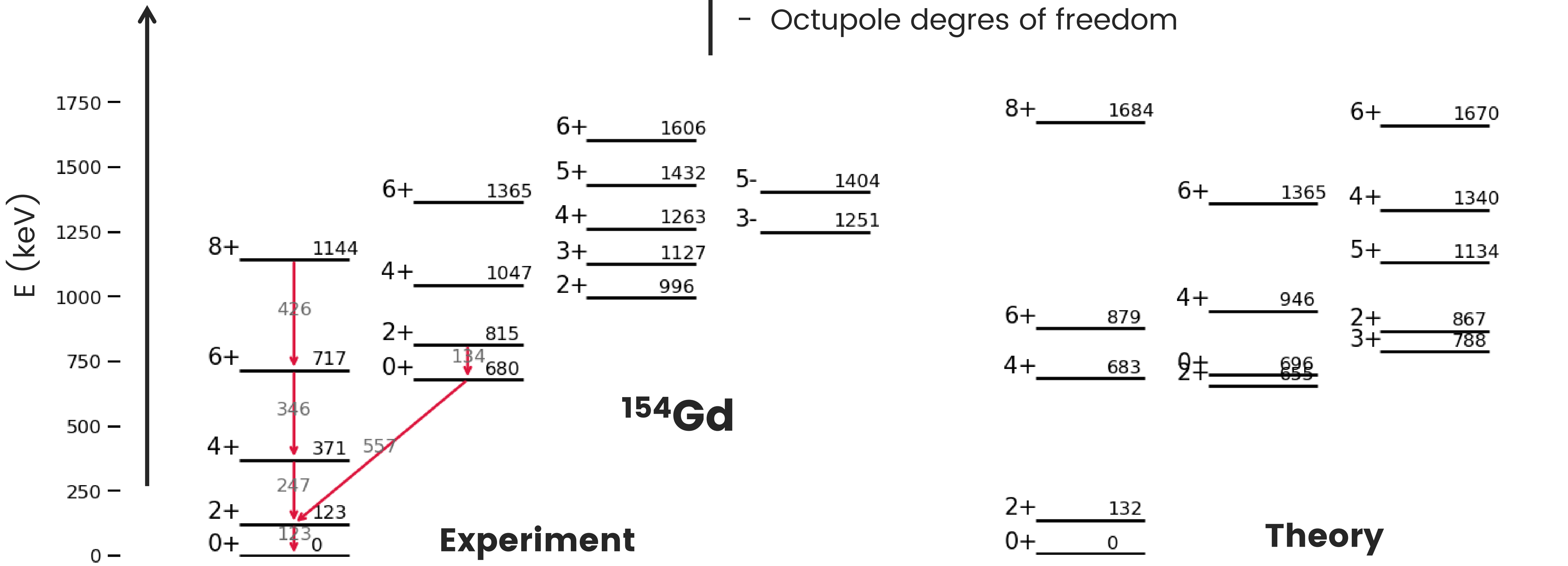


[ENSDF database, IAEA, https://www-nds.iaea.org/](https://www-nds.iaea.org/)

^{154}Gd spectrum

Improvement points :

- Zero point energy
- Mass calculation method: LQRPA, crancking
- Octupole degres of freedom



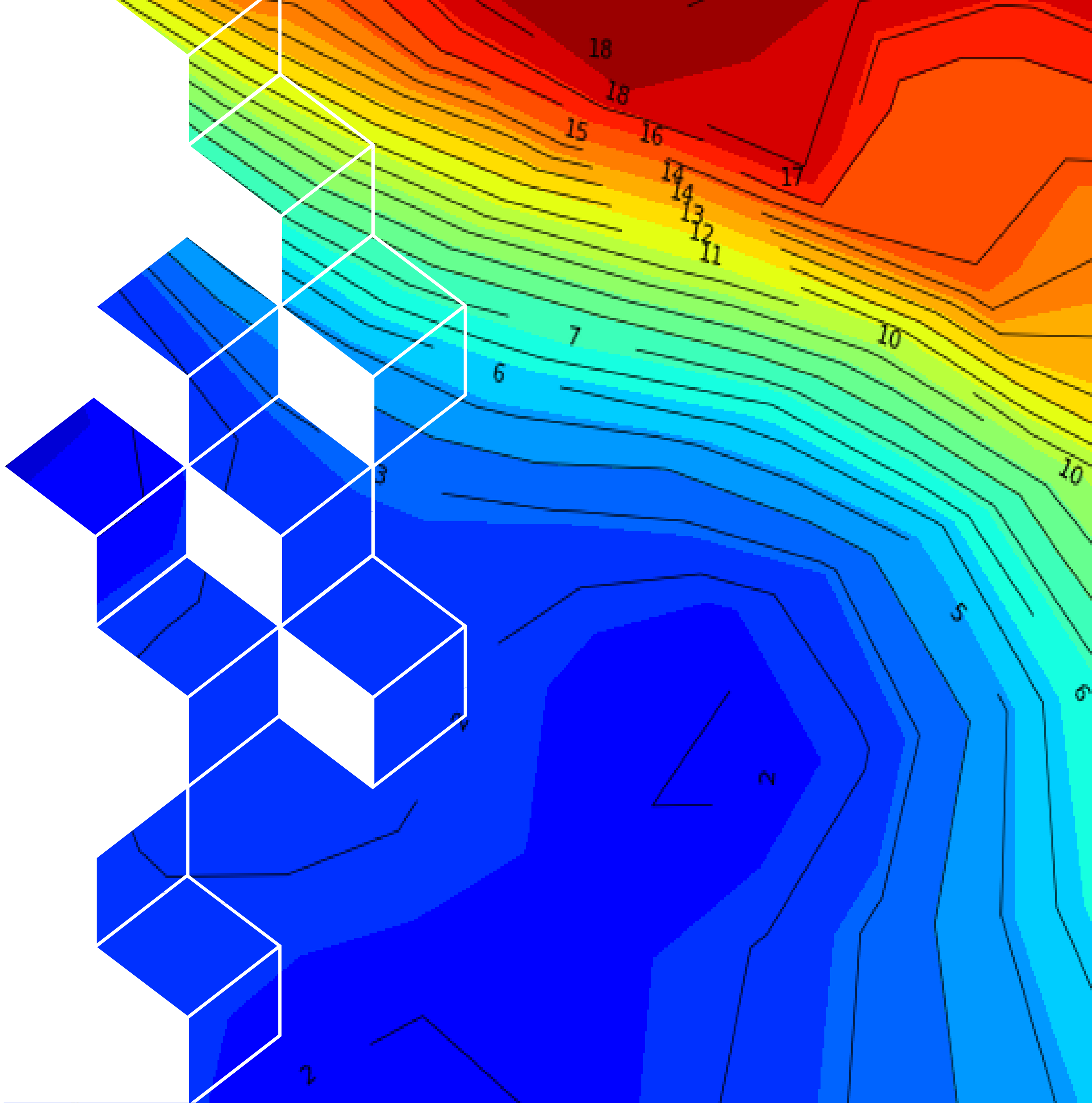
ENSDF database, IAEA, https://www-nds.iaea.org/

Conclusions et perspectives

- ✓ Quadrupole Bohr Hamiltonian formalism
- ✓ Quadrupole Bohr Hamiltonian code

- ❑ Improve the quadrupole results
- ❑ Addition of octupole degrees of freedom

Thank you for your attention

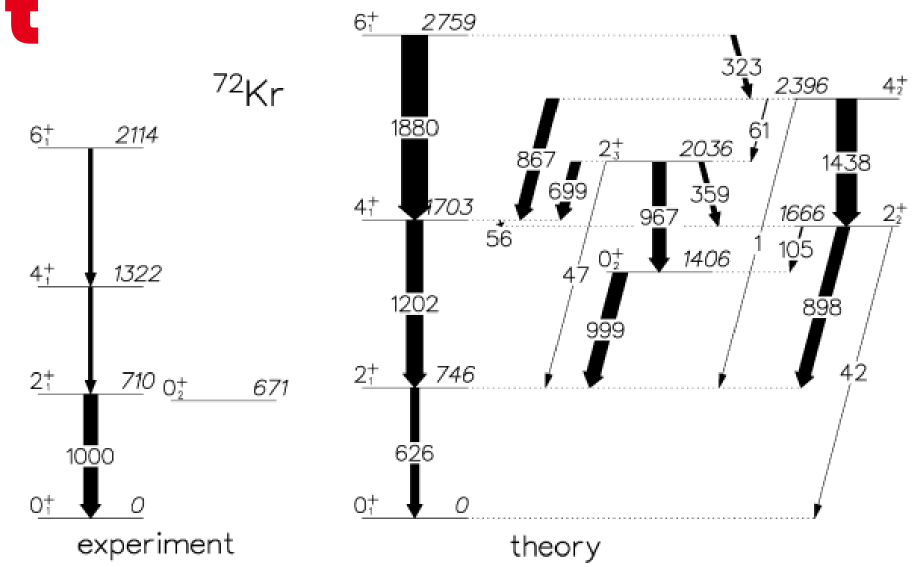


Ideas of improvment

Improvement points :

- Zero point energy

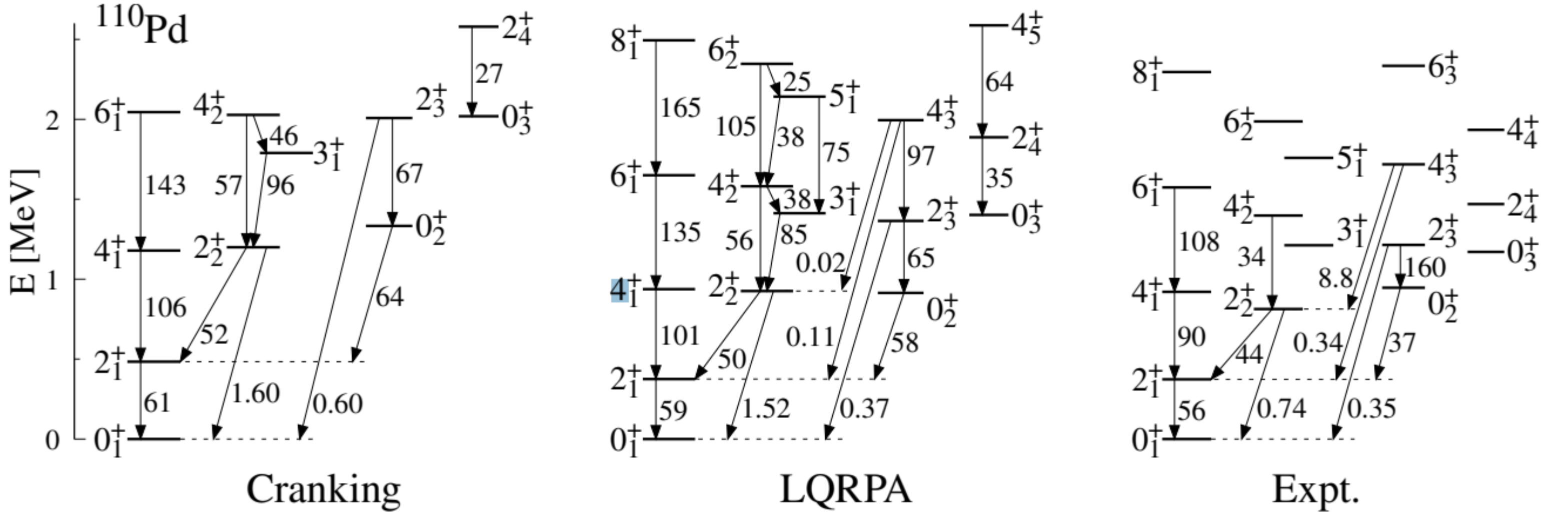
- Mass calculation method: LQRPA, crancking



[The role of triaxiality for the coexistence and evolution of shapes in light krypton isotopes – M.Girod et all. - 2024]

plus mu est grand et plus la fonction est localisée

[Five-dimensional collective Hamiltonian with improved inertial functions – K. Washiyama et al. - 2024]



Cranking approximation

Perturbative cranking :

$$B_{ij}(q) = \frac{\hbar^2}{2} \frac{M_{-3}^{ij}(q)}{[M_{-1}^{ij}(q)]^2}$$

$$M_{-k}^{ij}(q) = \sum_{\mu\nu} \frac{|\langle\phi|\eta_\mu\eta_\nu\hat{Q}_i|\phi\rangle\langle\phi|\eta_\mu\eta_\nu\hat{Q}_j|\phi\rangle|}{(E_\mu + E_\nu)^k}$$

η_μ Quasiparticle destruction operators
$\hat{Q}_i$ Quadrupole operators
q Quadrupolar collective coordinates
E_μ Quasiparticles energies