Ab-initio description of monopole resonances in light- and medium-mass nuclei

Preliminary results

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December 8, 2021
École Thématique PhyNuBe, Aussois

Outline

- Introduction
- Formalism
- Preliminary results
- Conclusions

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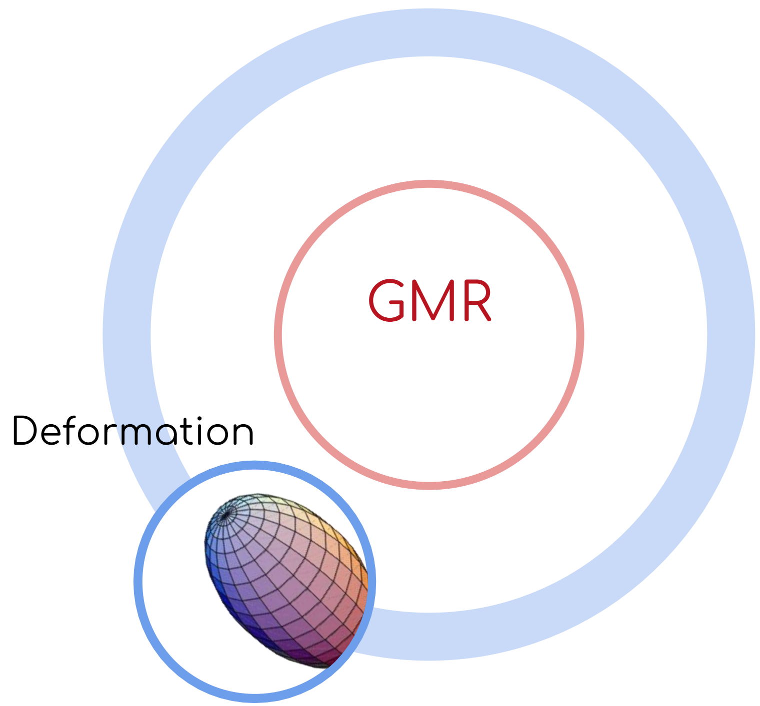

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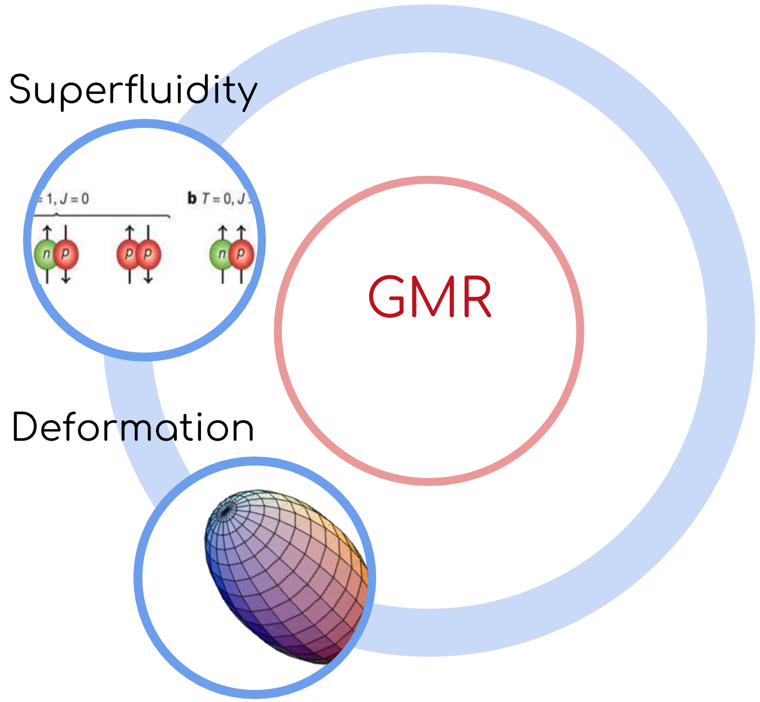

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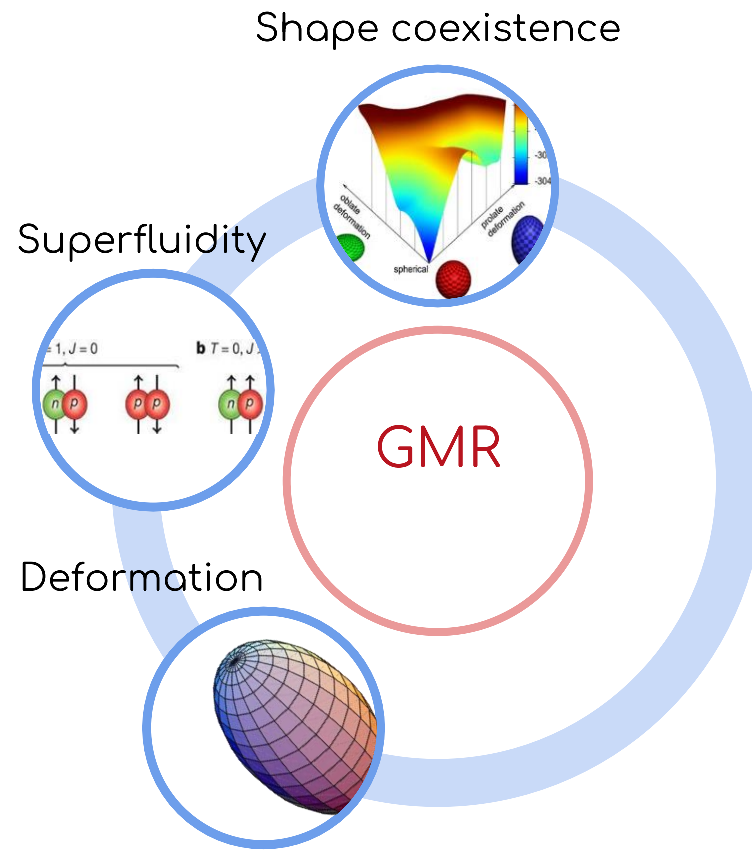

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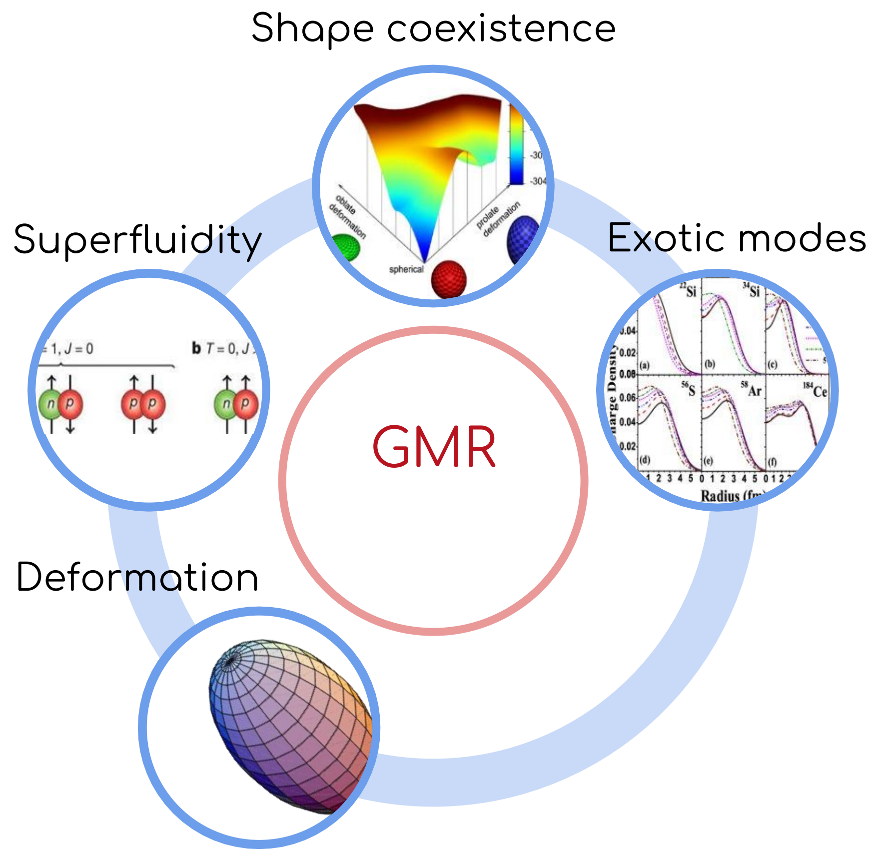

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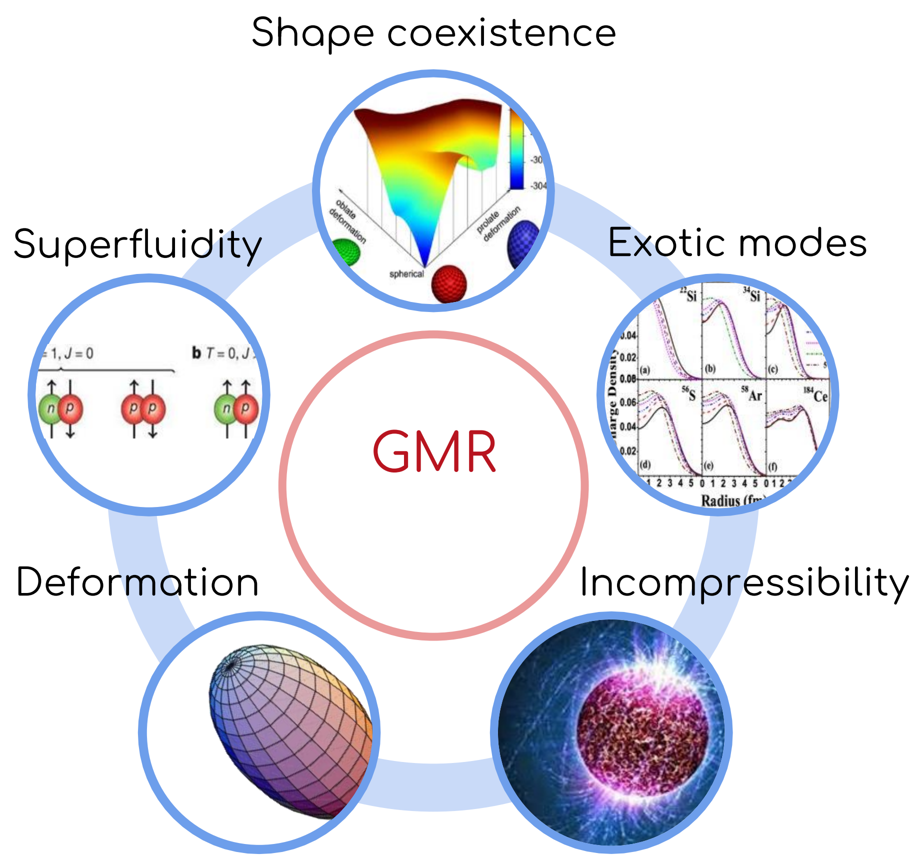

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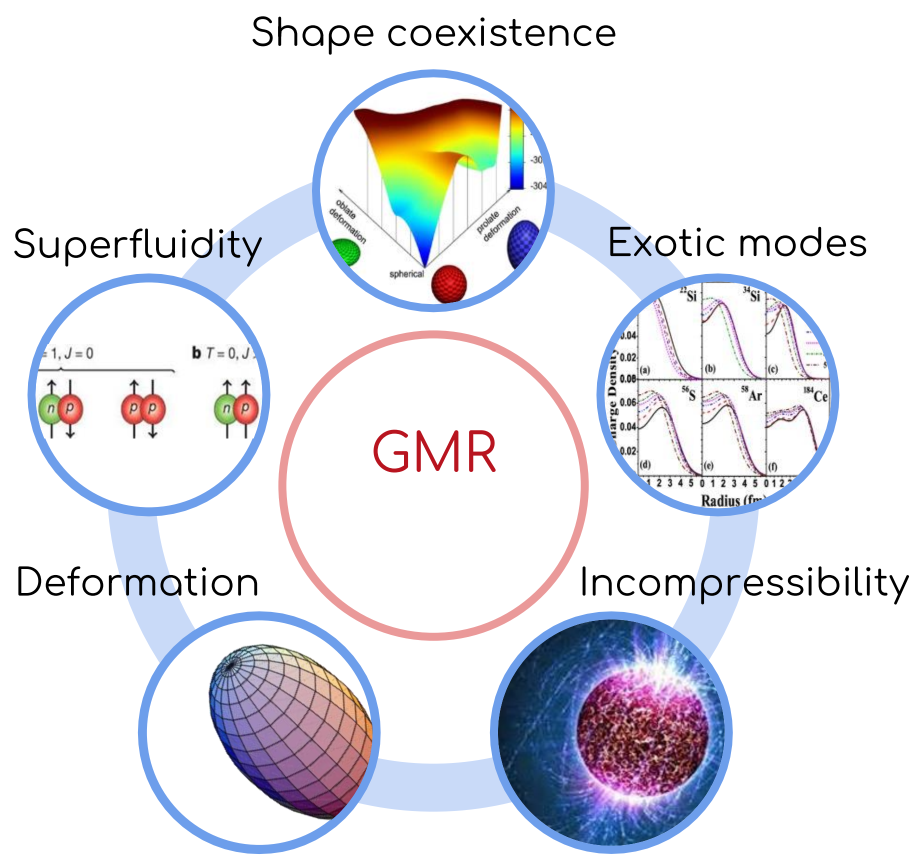
- No systematic studies (EDF as well)
  - Very generic numerical codes needed
- **Ab-initio description still seminal**



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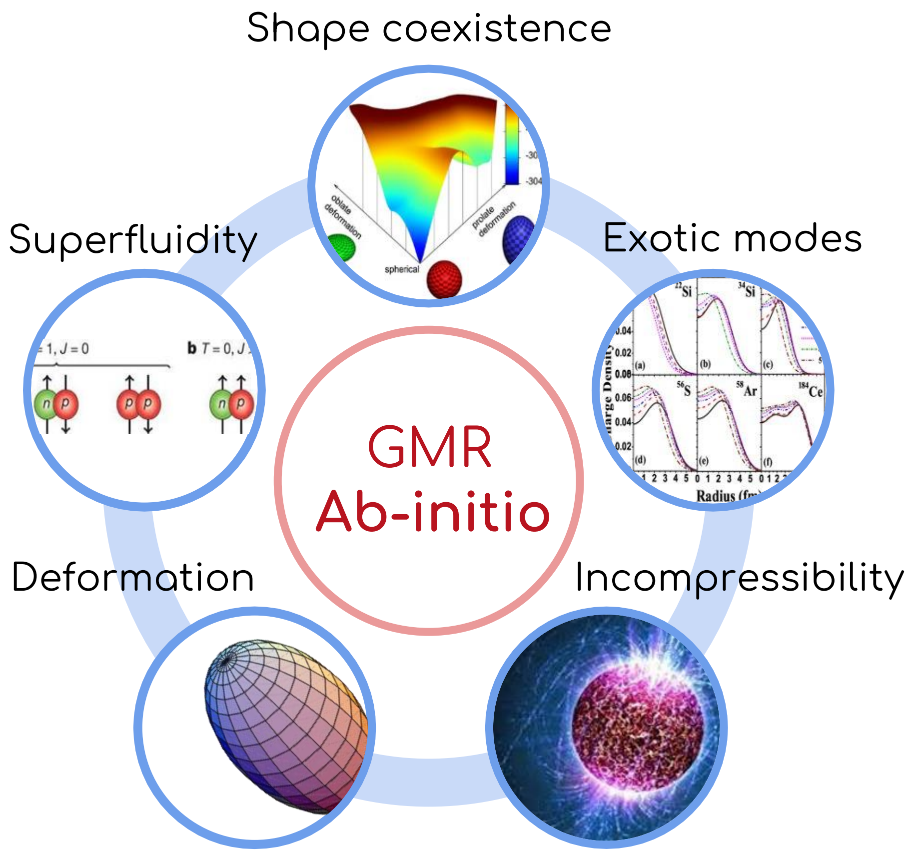

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Ab-initio methods

- *Ab-initio* methods have previously been introduced (see A. Tichai's and P. Demol's talks)
- Differences with Energy Density Functionals (EDF) theory

$$H|\Psi_\nu\rangle = E_\nu |\Psi_\nu\rangle$$

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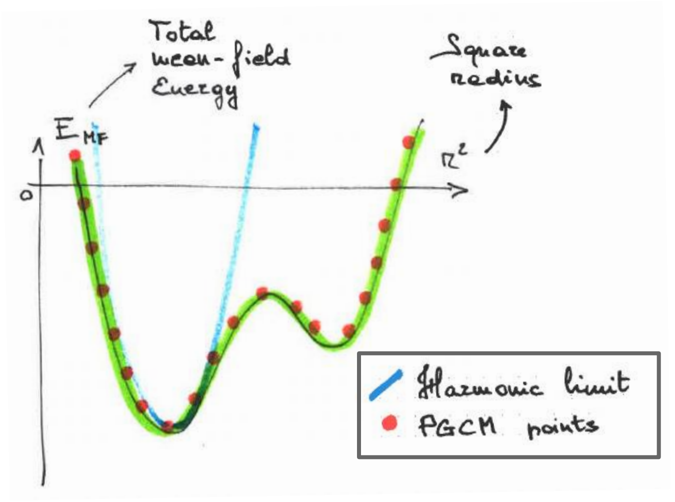
- PGCM (Projected GCM)
- QFAM (QRPA implementation)

PGCM vs QRPA

Schrödinger equation $$H\left|\Psi_\nu\right\rangle = E_\nu \left|\Psi_\nu\right\rangle$$



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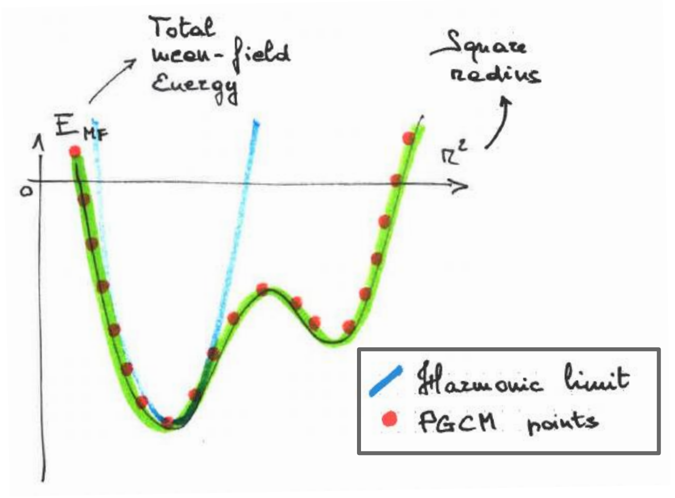
$$|\Psi_\nu\rangle \equiv \sum_{r^2,q} f_\nu(r^2,q)\,|\Phi(r^2,q)\rangle$$

r^2 to study GMR

q to couple to other modes

Symmetry breaking and restoration

Variational method



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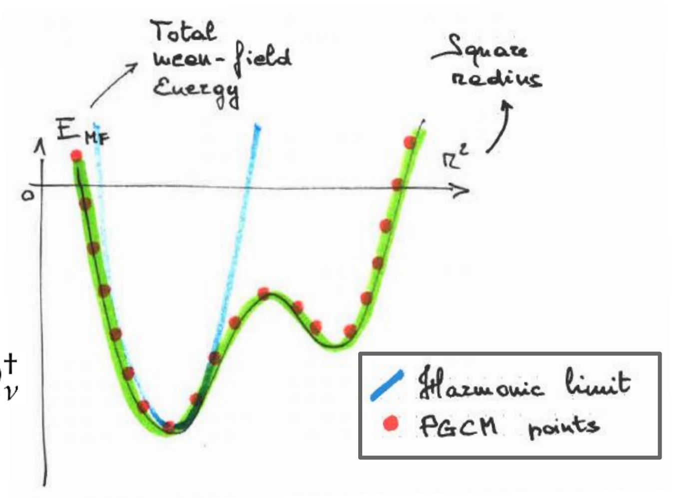
QRPA matrix diagonalization

QFAM formulation frequencies $\mathbb{C}$



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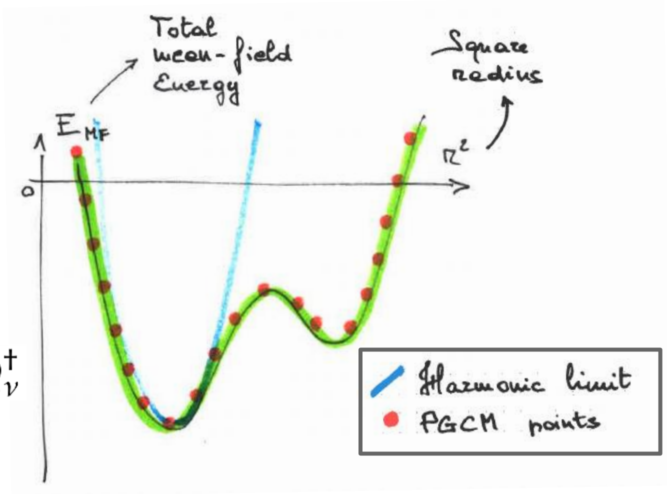

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Handle anharmonicities and shape coexistance	Harmonic limit of GCM
Select on few collective coordinates	All coordinates are explored
Symmetries are restored	Symmetries are not restored
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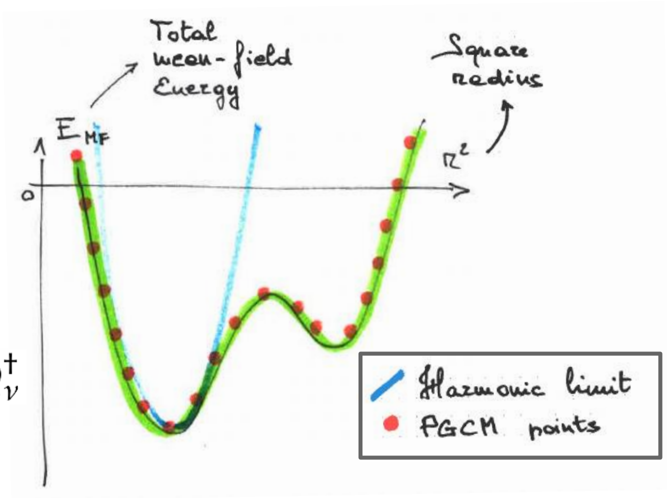

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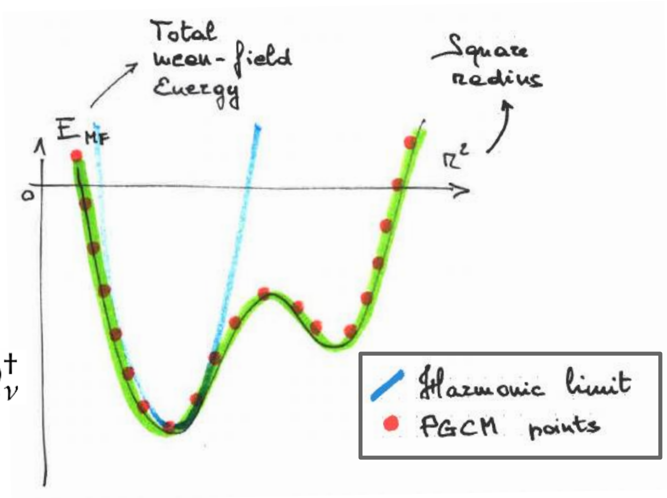

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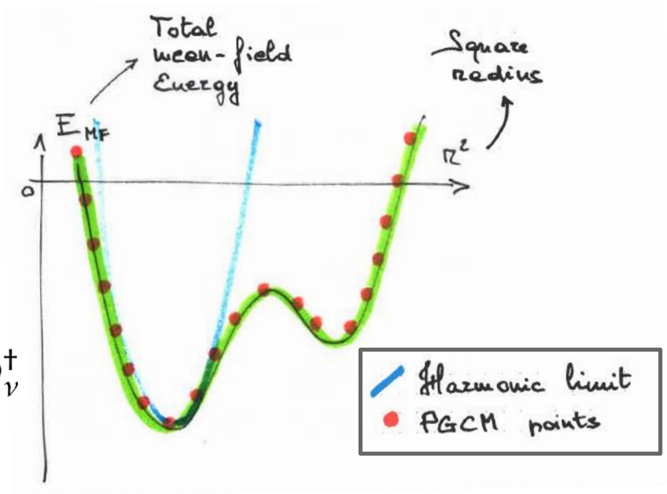

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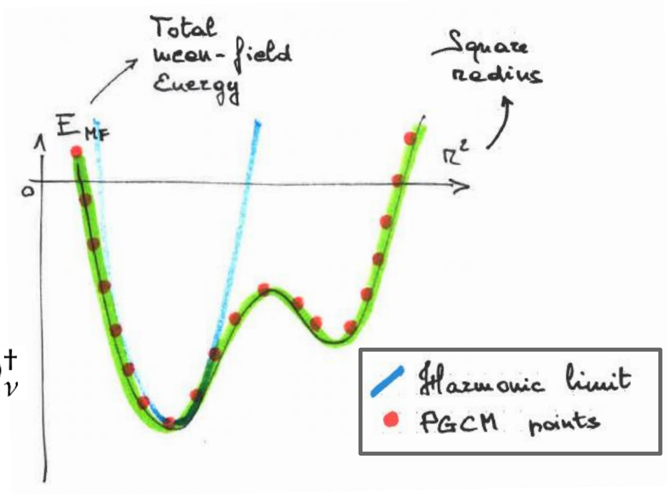

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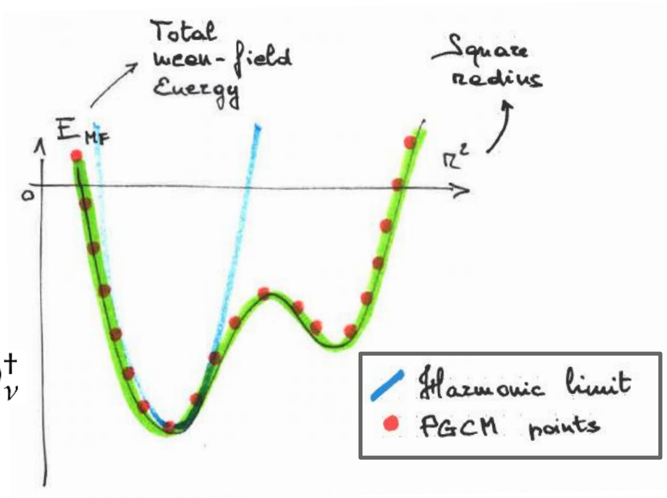

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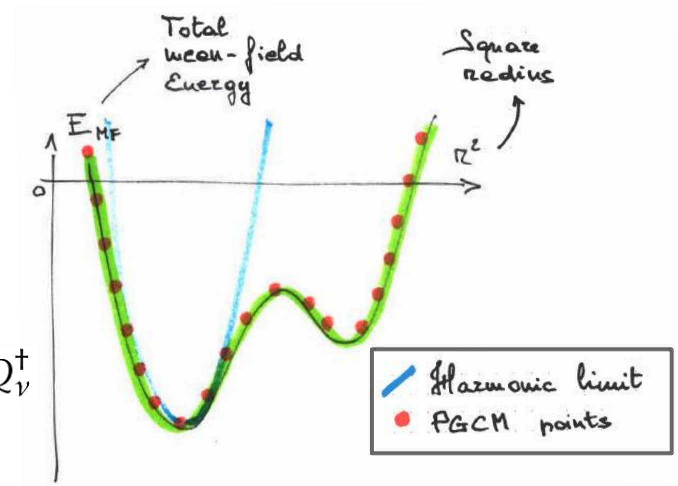

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General implementation, can access

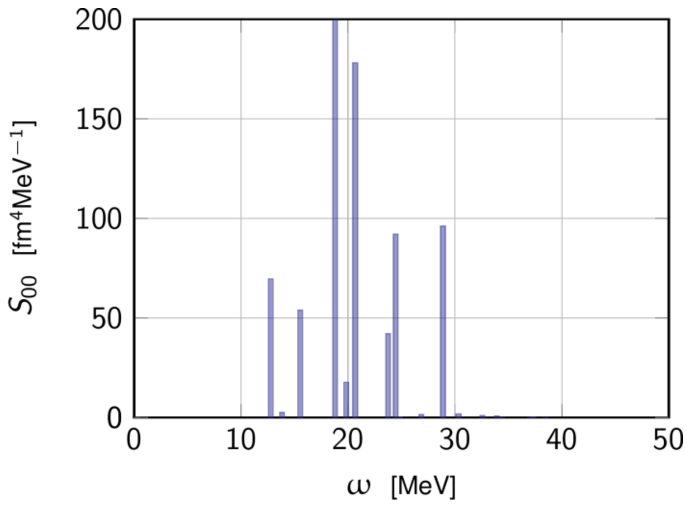
1. Doubly-closed-shell nuclei
2. Singly-open-shell nuclei
3. Doubly-open-shell nuclei

Moments and Strength

- Studied quantity: monopole strength

$$S_{00}(\omega) \equiv \sum_{\nu} |\langle \Psi_\nu | r^2 | \Psi_0 \rangle|^2 \delta(E_\nu - E_0 - \omega)$$

  - Transition amplitudes: height of peaks
  - Energy difference: position of peaks



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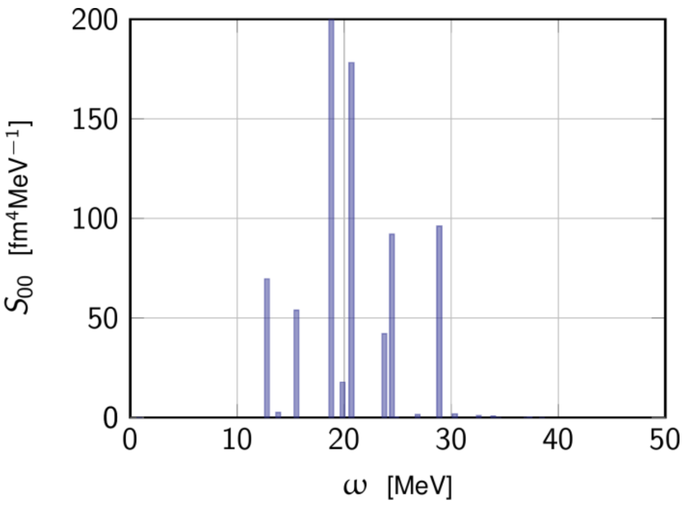

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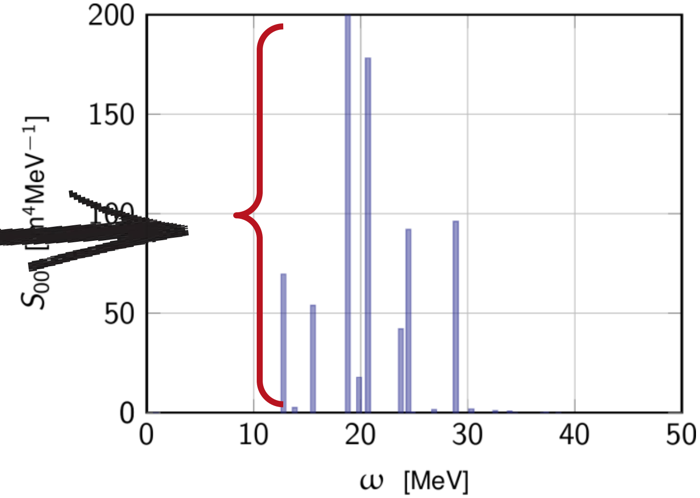

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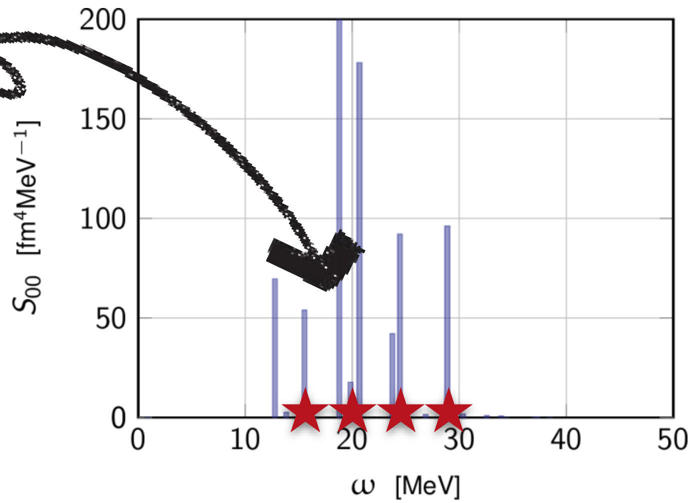

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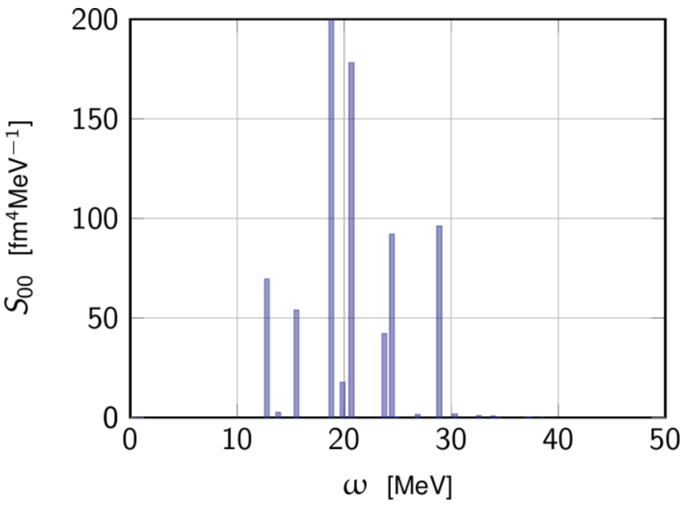

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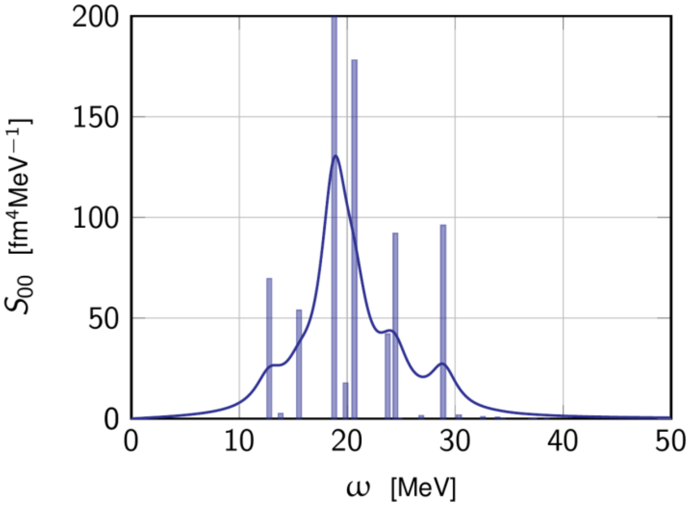

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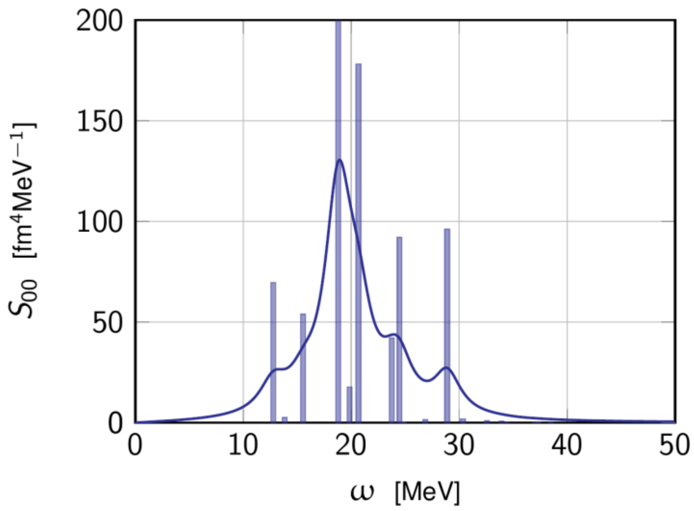
- Related moments

$$\begin{aligned} m_k &\equiv \int_0^\infty S_{00}(\omega)\, \omega^k \, d\omega \\ &= \sum_{\nu} (E_\nu - E_0)^k |\langle \Psi_\nu | r^2 | \Psi_0 \rangle|^2 \\ &\equiv \langle \Psi_0 | \check{M}_k(i,j) | \Psi_0 \rangle \end{aligned}$$



[Bohigas et al., 1979]

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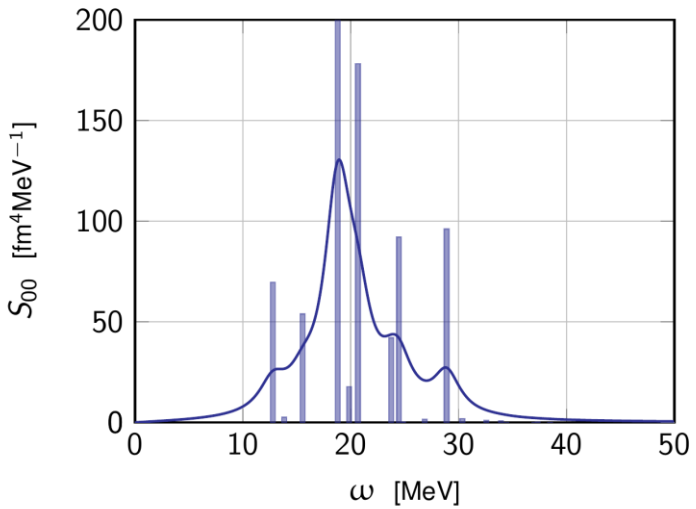

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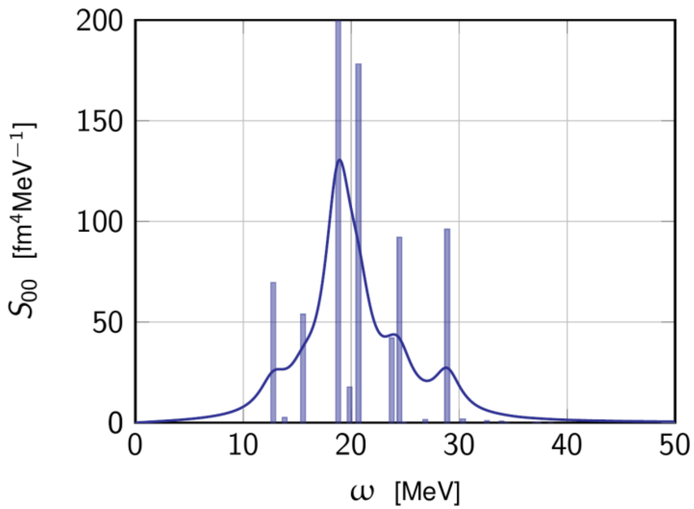

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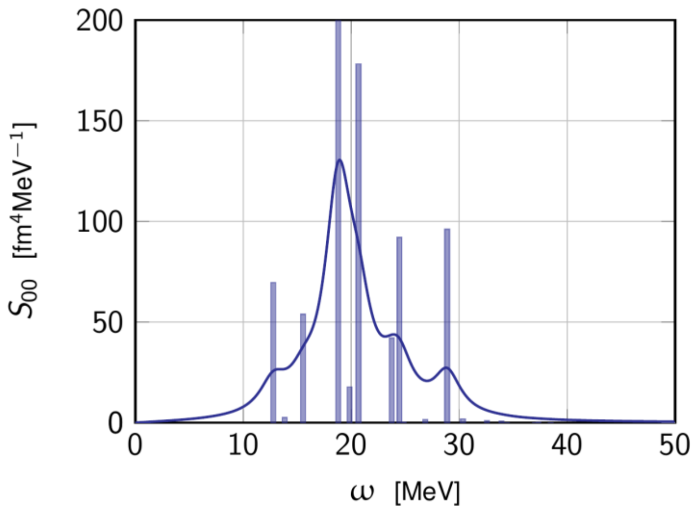

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[Bohigas et al., 1979]

Complexity is shifted to the operator structure

$$\breve{M}_k(i,j) \equiv (-1)^i C_i C_j \qquad \forall\ k \geq 0$$

$$M_k(i,j) \equiv \frac{1}{2}(-1)^i [C_i, C_j] \ \text{ if } \ k = 2n+1, \quad n \in \mathbb{N}$$

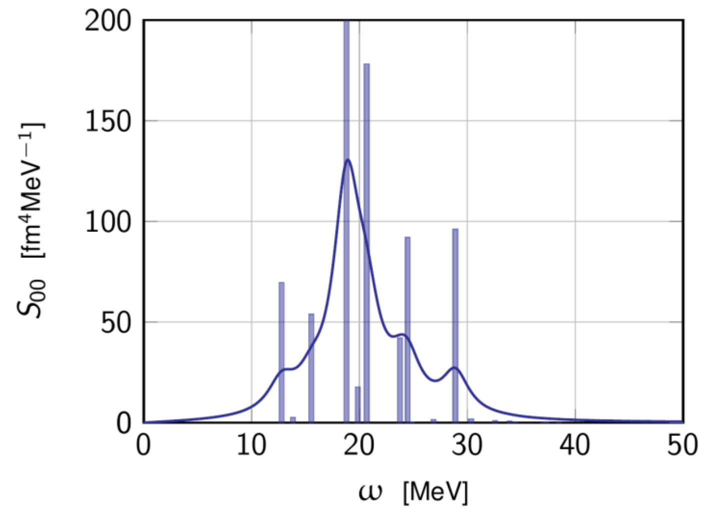
$$C_l \equiv \underbrace{[H,[H,\ldots[H,[H}_{l \text{ times}},r^2]]\ldots]]$$

Moments and Strength

- Studied quantity: monopole strength

$$S_{00}(\omega) \equiv \sum_{\nu} |\langle \Psi_\nu | r^2 | \Psi_0 \rangle|^2 \delta(E_\nu - E_0 - \omega)$$

  - Transition amplitudes: height of peaks
  - Energy difference: position of peaks



- Related moments $m_k \equiv \int_0^\infty S_{00}(\omega)\, \omega^k \, d\omega$

$$= \sum_\nu (E_\nu - E_0)^k |\langle \Psi_\nu | r^2 | \Psi_0 \rangle|^2 \longrightarrow \text{Must know excited states}$$

$$\equiv \langle \Psi_0 | \breve{M}_k(i,j) | \Psi_0 \rangle \longrightarrow \text{Ground state only}$$

[Bohigas et al., 1979]

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Encode the main physical features of the strength

$$\boxed{\bar{E}_1 = \frac{m_1}{m_0} \qquad \sigma^2 = \frac{m_2}{m_0} - \left(\frac{m_1}{m_0}\right)^2 \geq 0}$$

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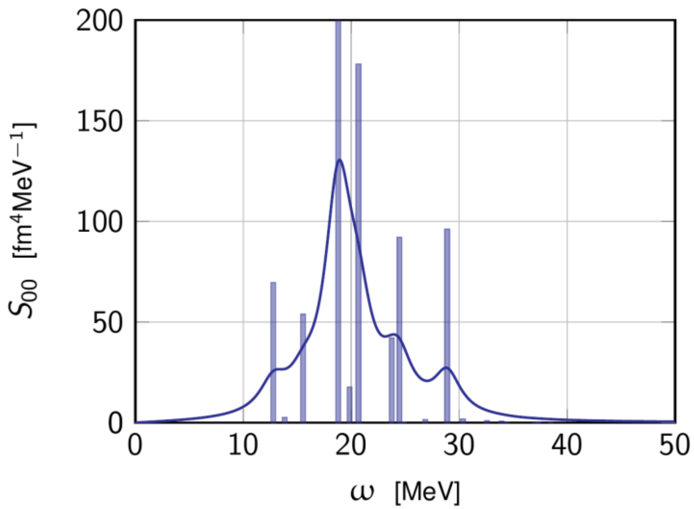

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First comparison ever of the two approaches !

Derived and **implemented** in an ab-initio PGCM code

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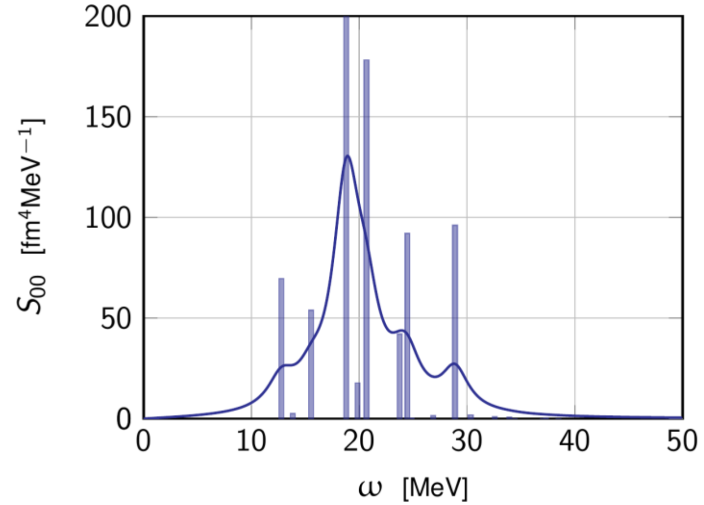

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First comparison ever of the two approaches !

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Not discussed in the present talk

Outline

- Introduction
- Formalism
- **Preliminary results**
- Conclusions

Common features

PGCM and QFAM have consistent numerical settings

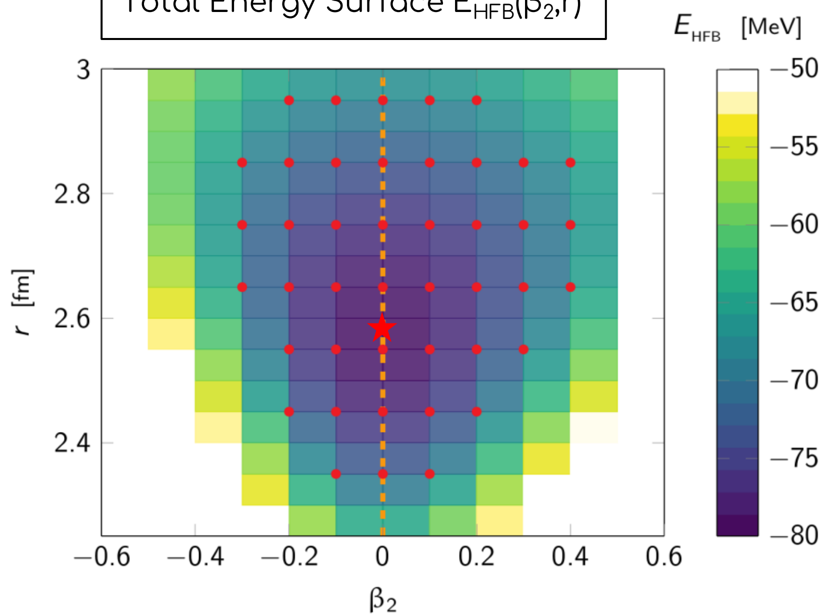
- One-body spherical harmonic oscillator basis
  - $e_{max} = 10$
  - $\hbar\omega = 20$ MeV
- Chiral two-plus-three-nucleon in-medium interaction
  - T. Hüther, K. Vobig, K. Hebeler, R. Machleidt and R. Roth, "Family of chiral two-plus three-nucleon interactions for accurate nuclear structure studies", *Phys. Lett. B,* 808, 2020
  - M. Frosini, T. Duguet, B. Bally, Y. Beaujeault-Taudière, J.-P. Ebran and V. Somà, “In-medium k-body reduction of n-body operators“, *The European Physical Journal A*, *57*(4), 2021
- **Only monopole strength is addressed**
- PGCM: GMR with quadrupole coupling (r^2 + β_2 collective coordinates)

Benchmarking ^{16}O

Difficulty

- ☐ Benchmark on existing spherical QRPA code

Total Energy Surface $E_{HFB}(\beta_2, r)$



Results

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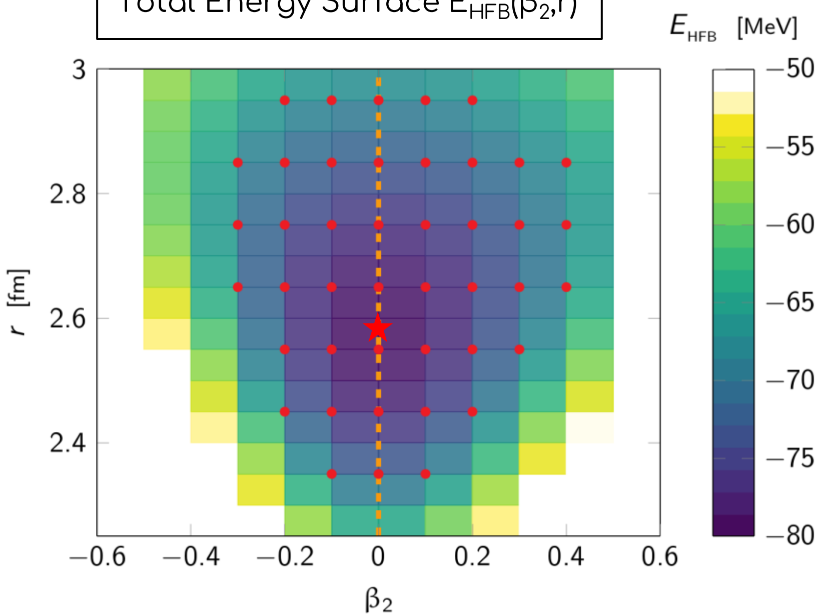
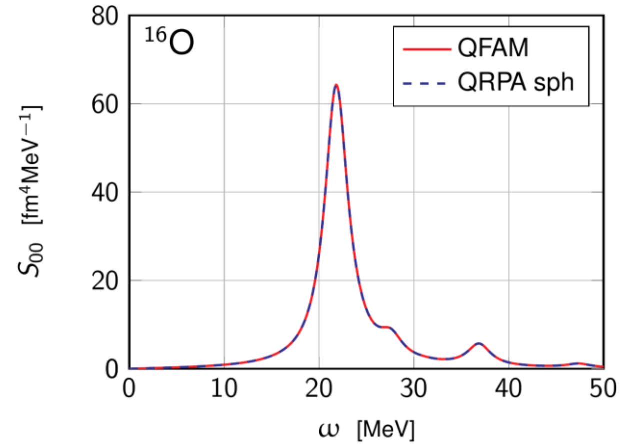


Monopole Strength



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- Single spherical harmonic energy minimum
- Exact QRPA/QFAM superposition

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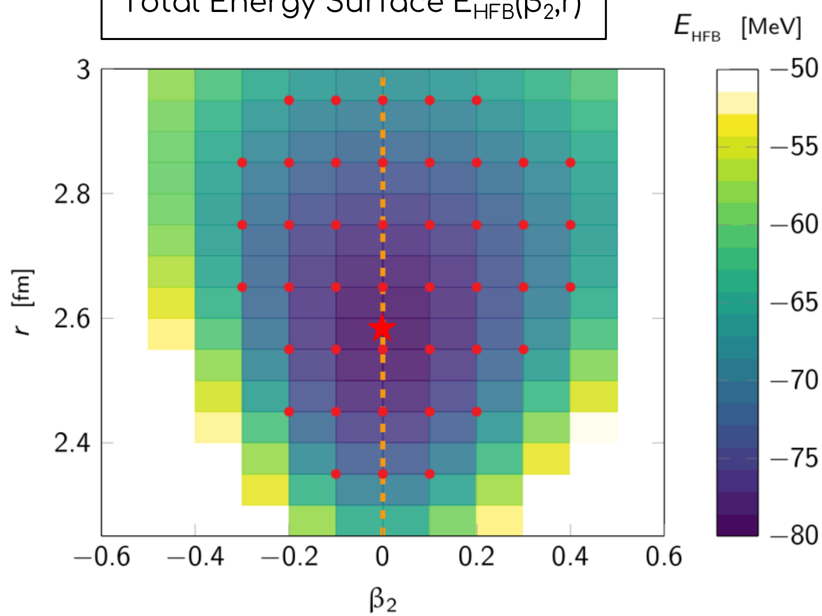

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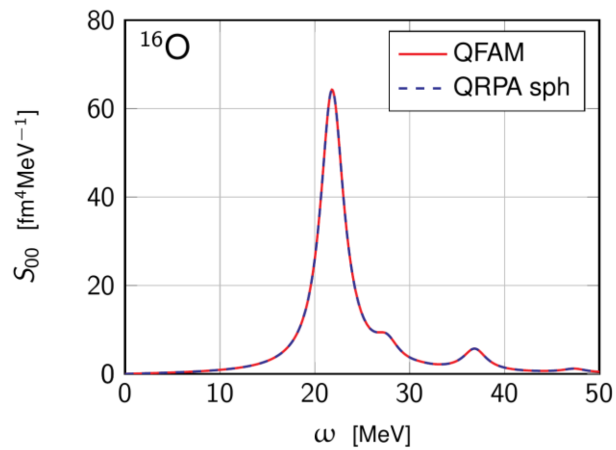

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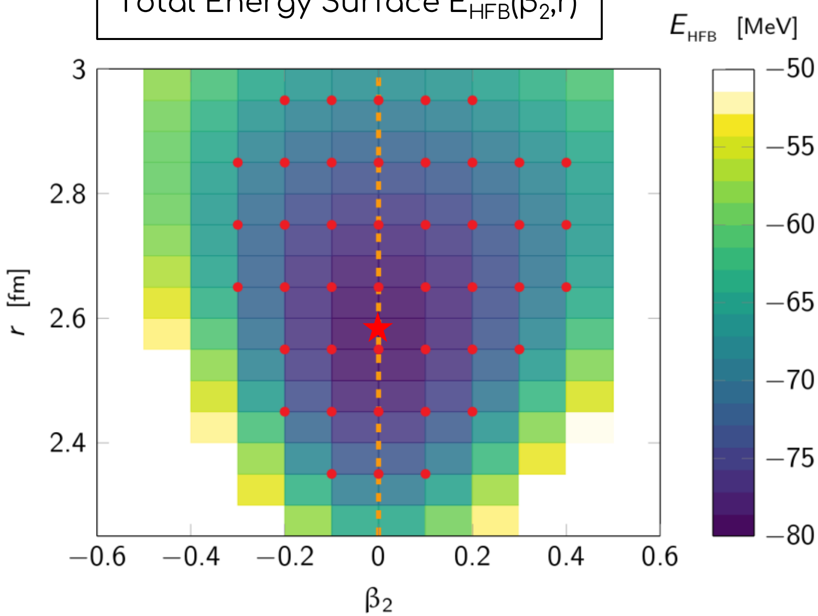

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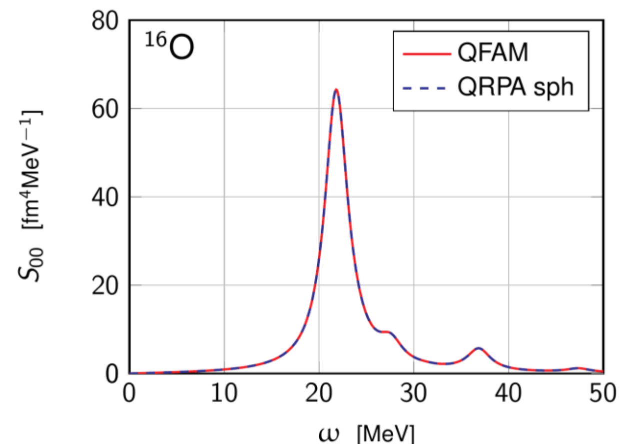

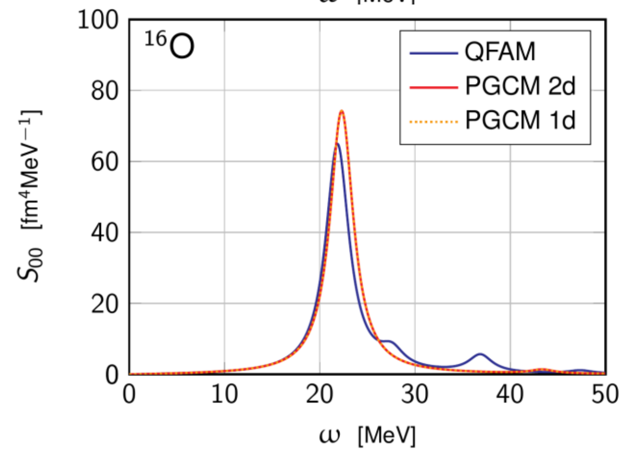

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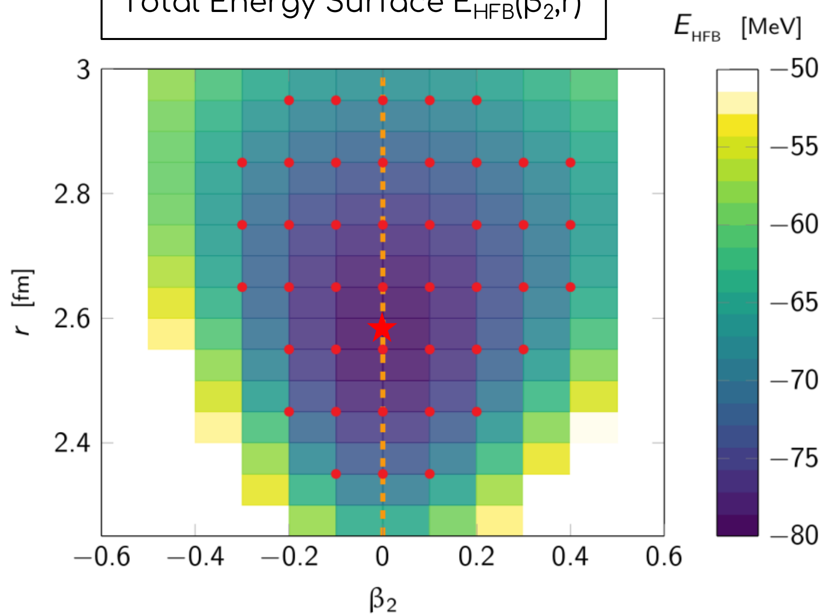

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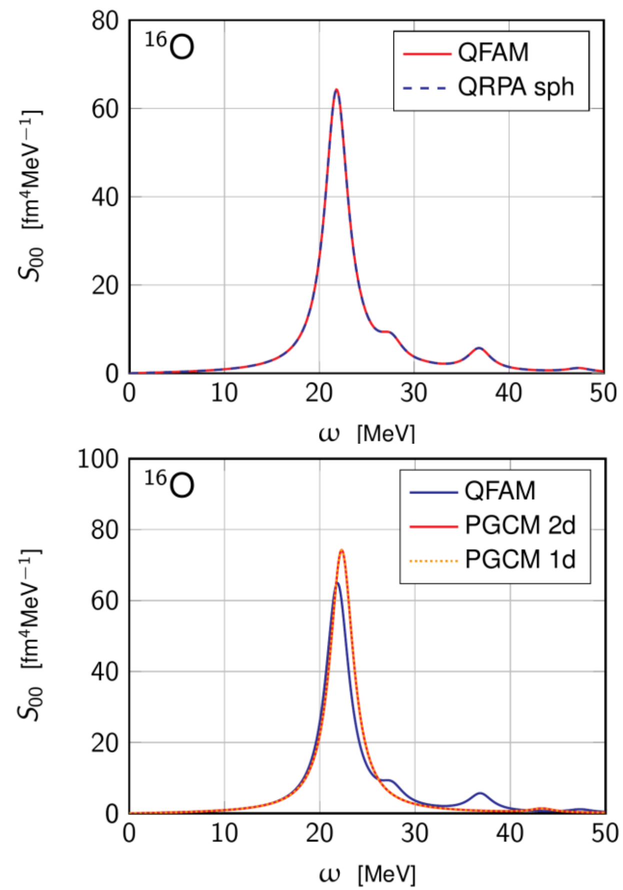

Results

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Benchmarking ^{16}O

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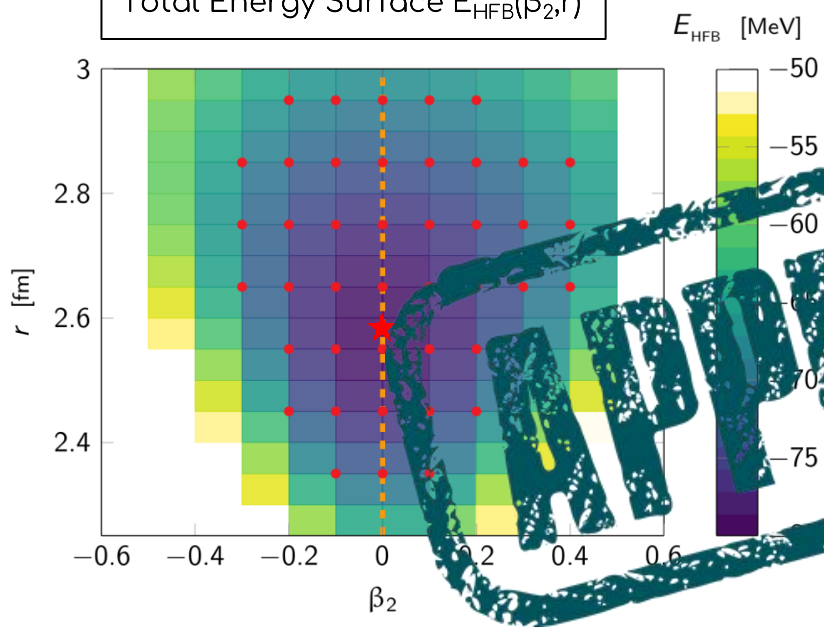

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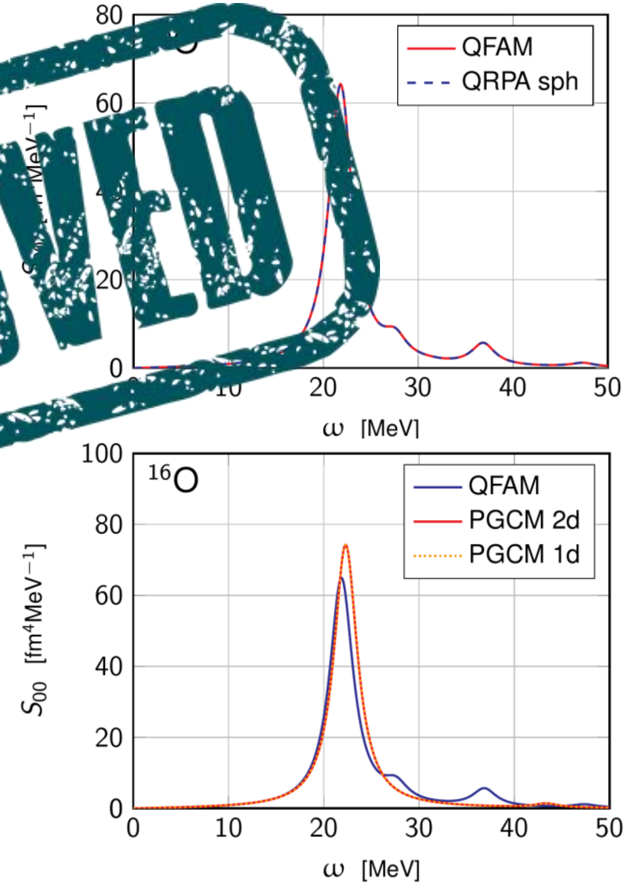

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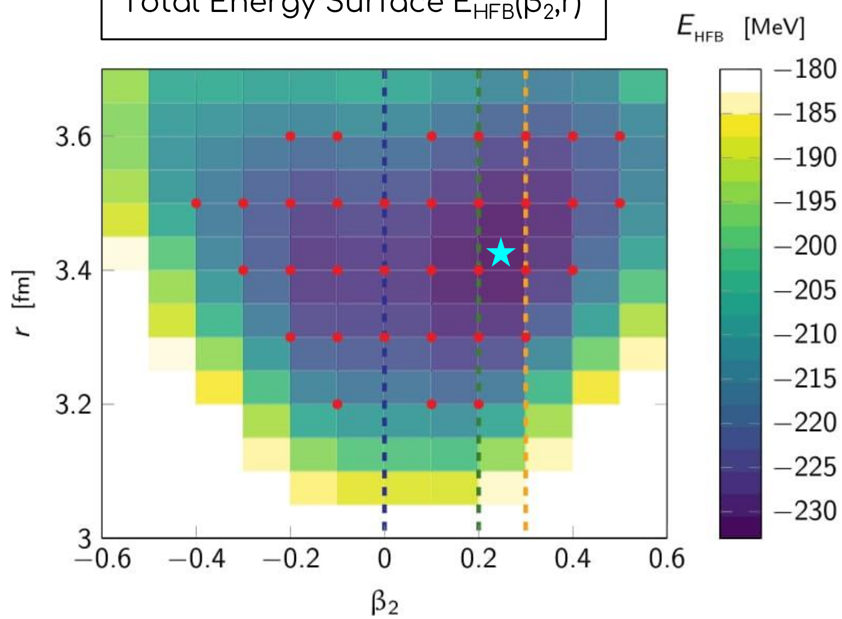
Deformation effects in ^{46}Ti

Difficulty

Total Energy Surface $E_{HFB}(\beta_2,r)$



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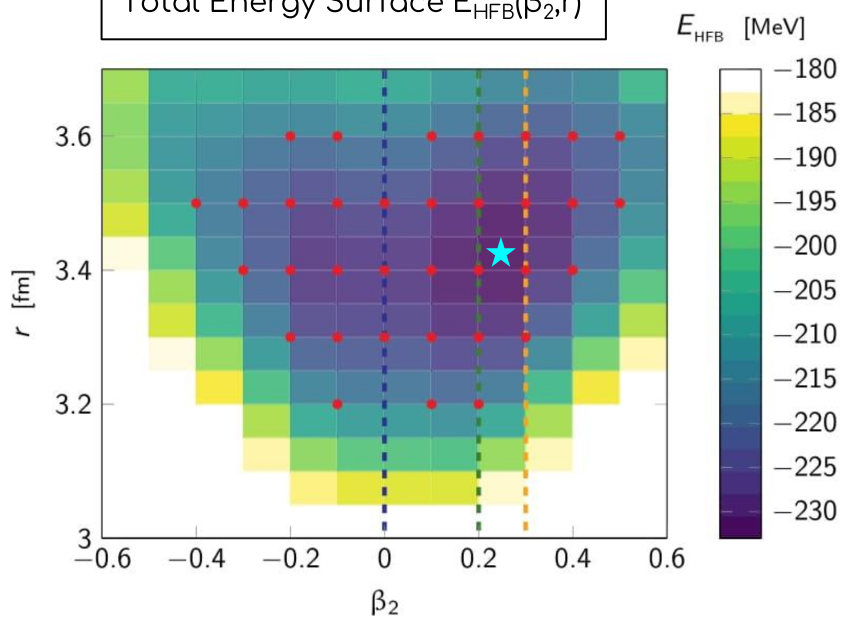

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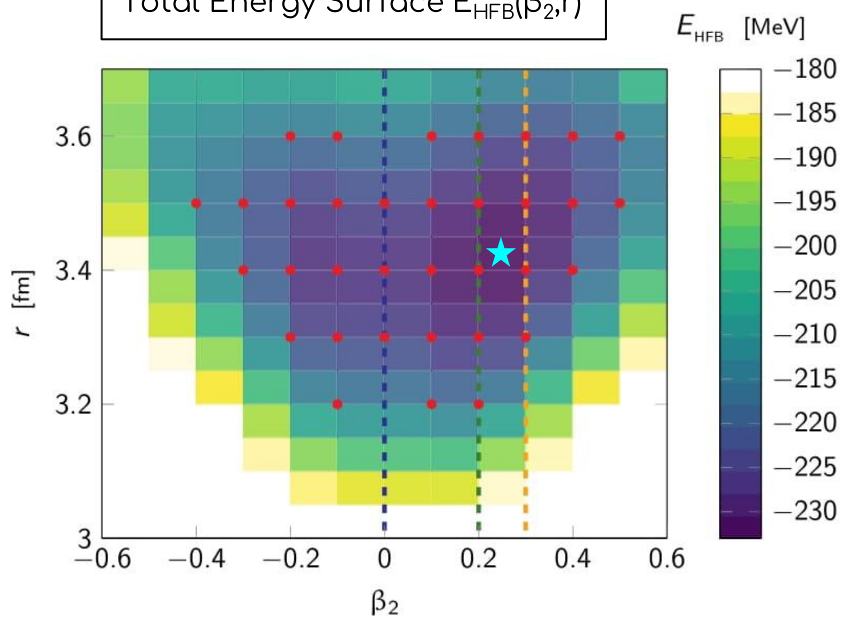

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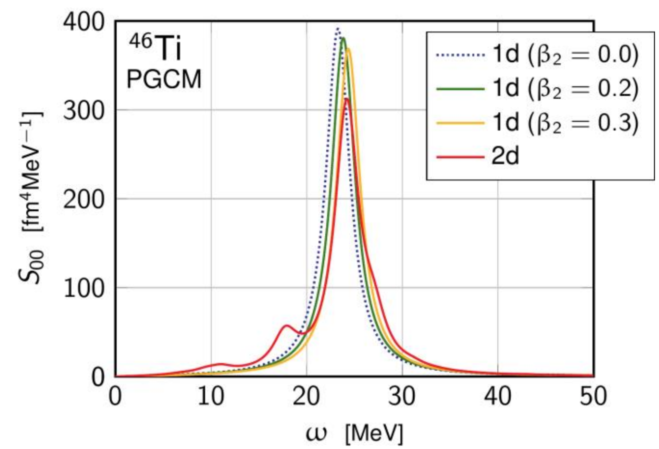

Results

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- Little effect of static quadrupole deformation

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Difficulty

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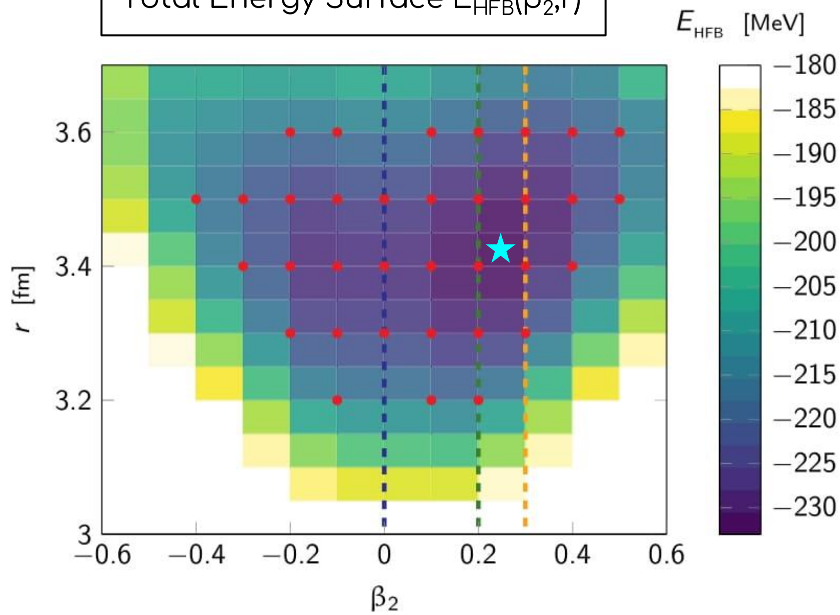

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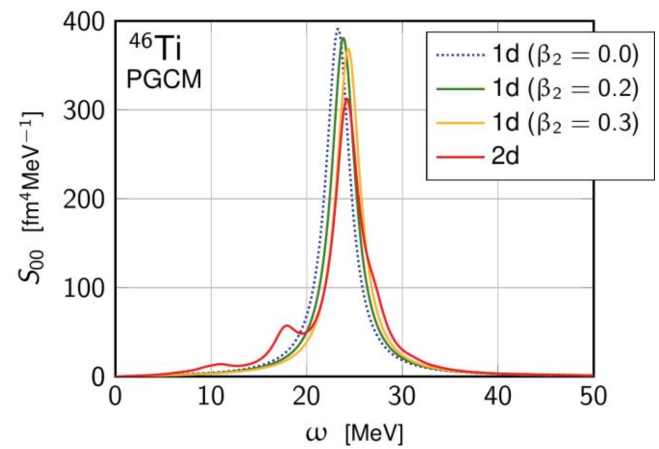

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- Little effect of static quadrupole deformation
- Weak coupling with quadrupolar vibrations

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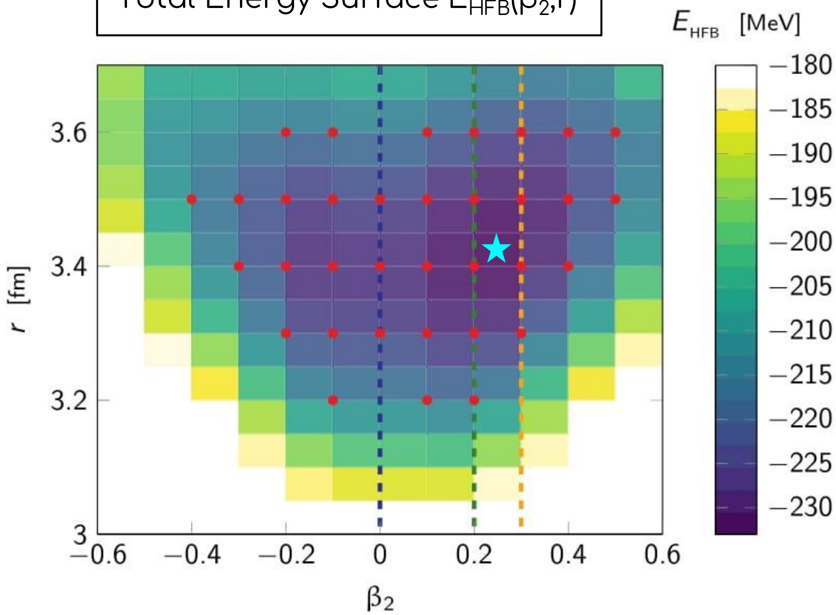

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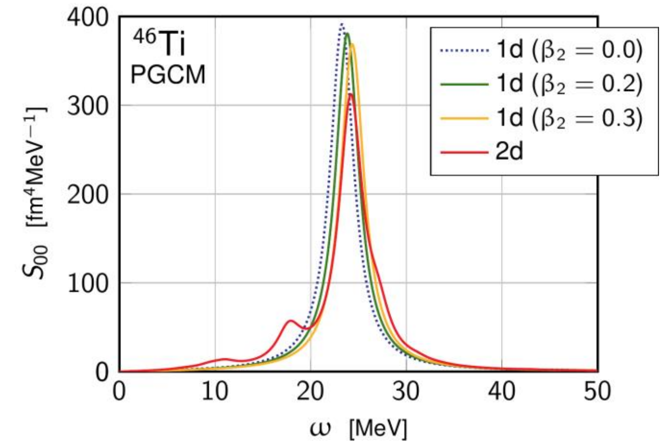
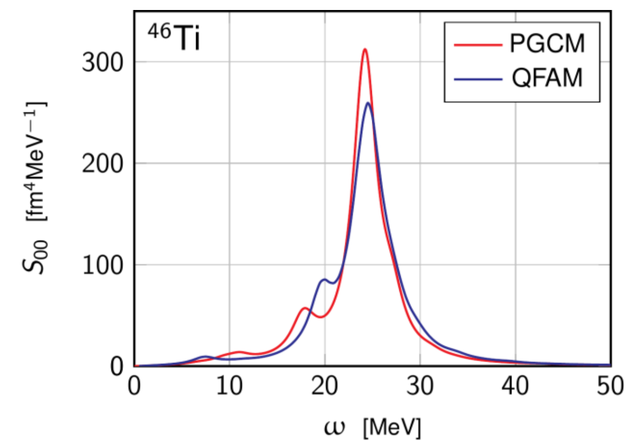




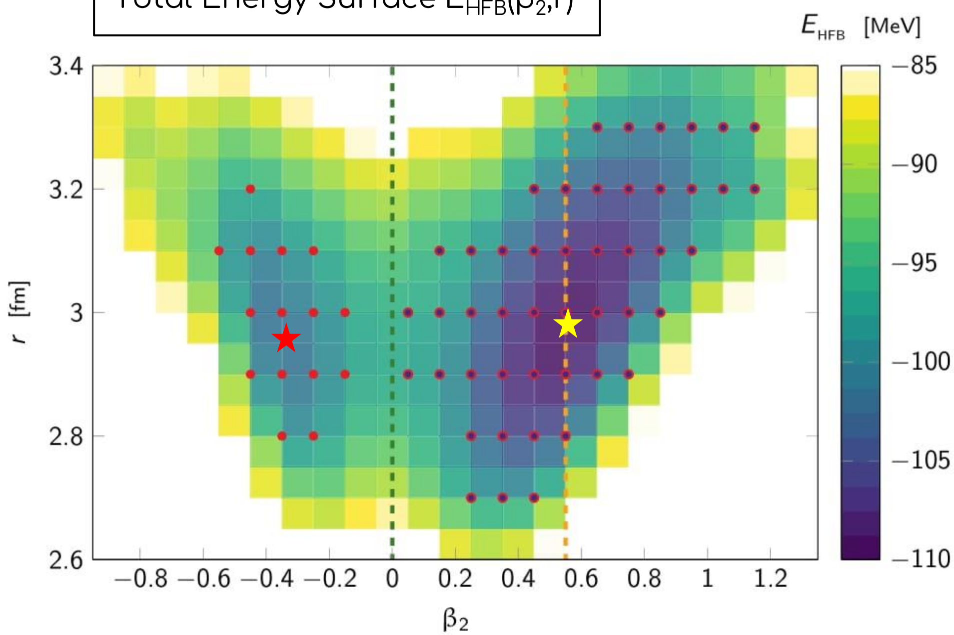
Results

- Single prolate minimum
- Little effect of static quadrupole deformation
- Weak coupling with quadrupolar vibrations
- Good QFAM/PGCM agreement

Deformation effects in ^{24}Mg

Difficulty

Total Energy Surface $E_{HFB}(\beta_2,r)$



Results

- Dominant prolate minimum

Deformation effects in ^{24}Mg

Difficulty

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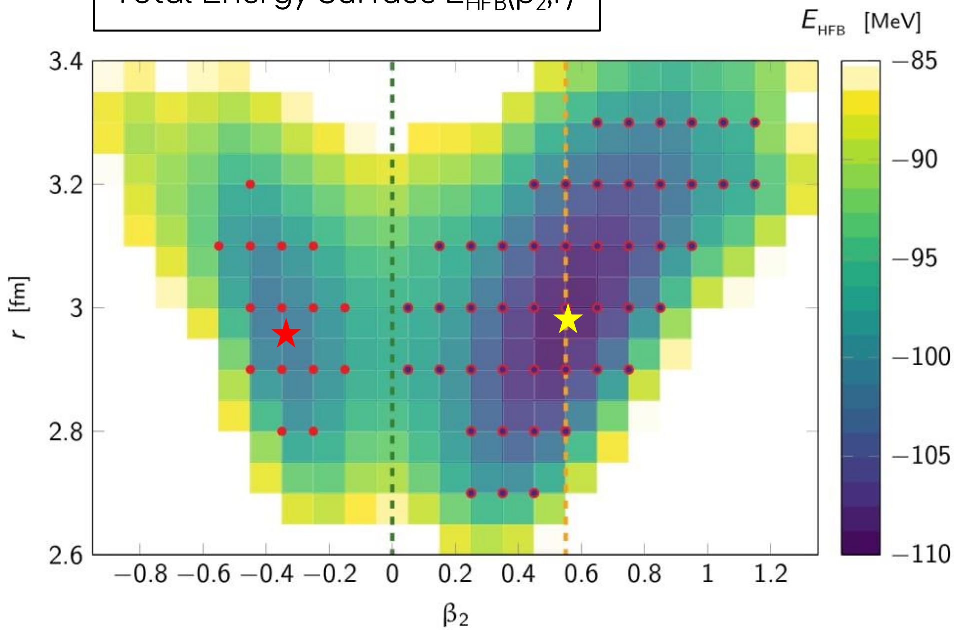

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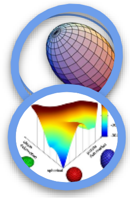

Deformation

Shape coexistence ? (1)

(1) [Dowie et al., 2020]

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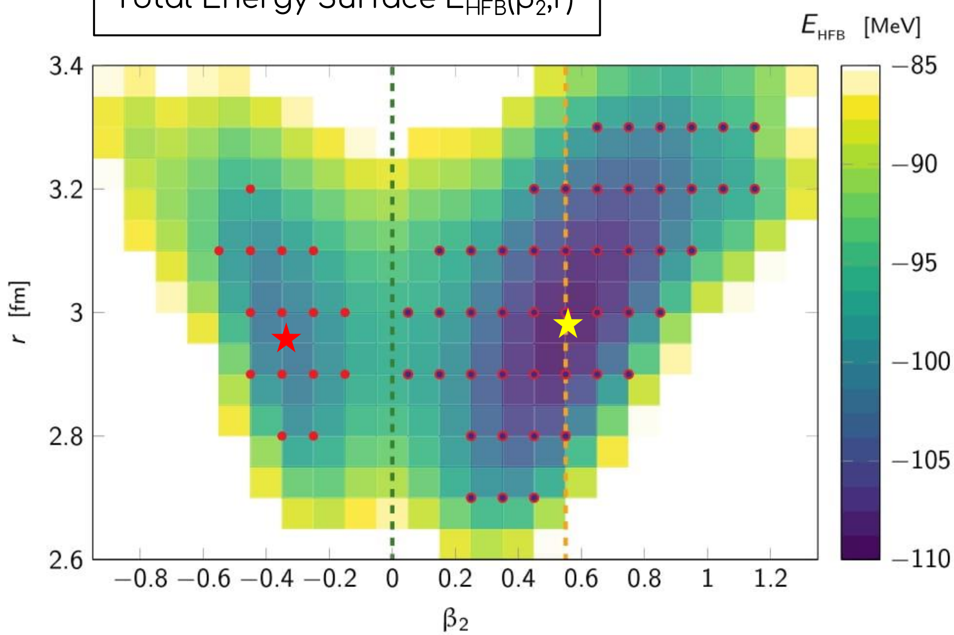

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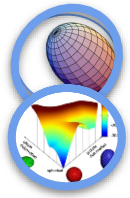

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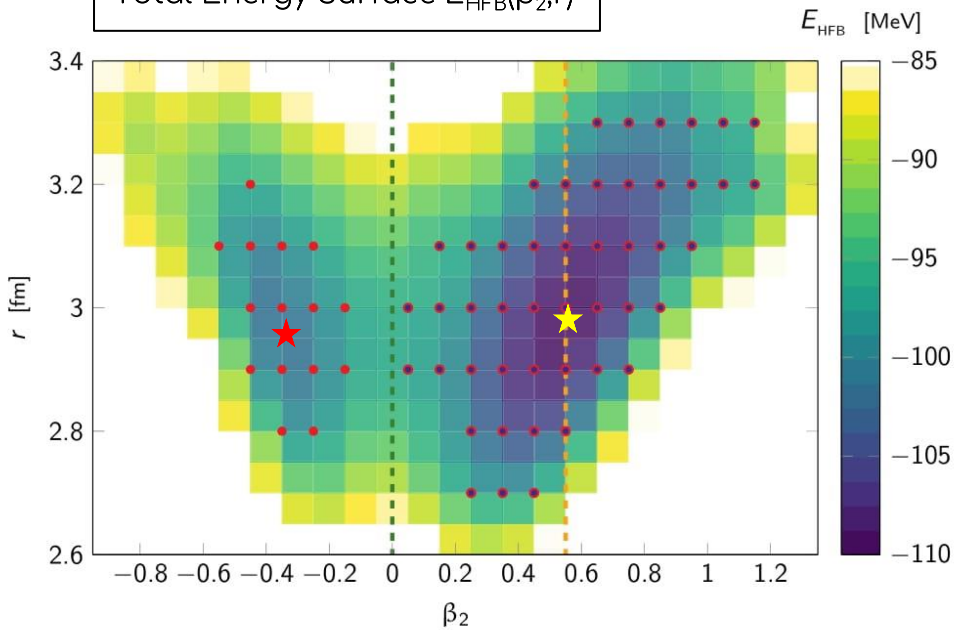

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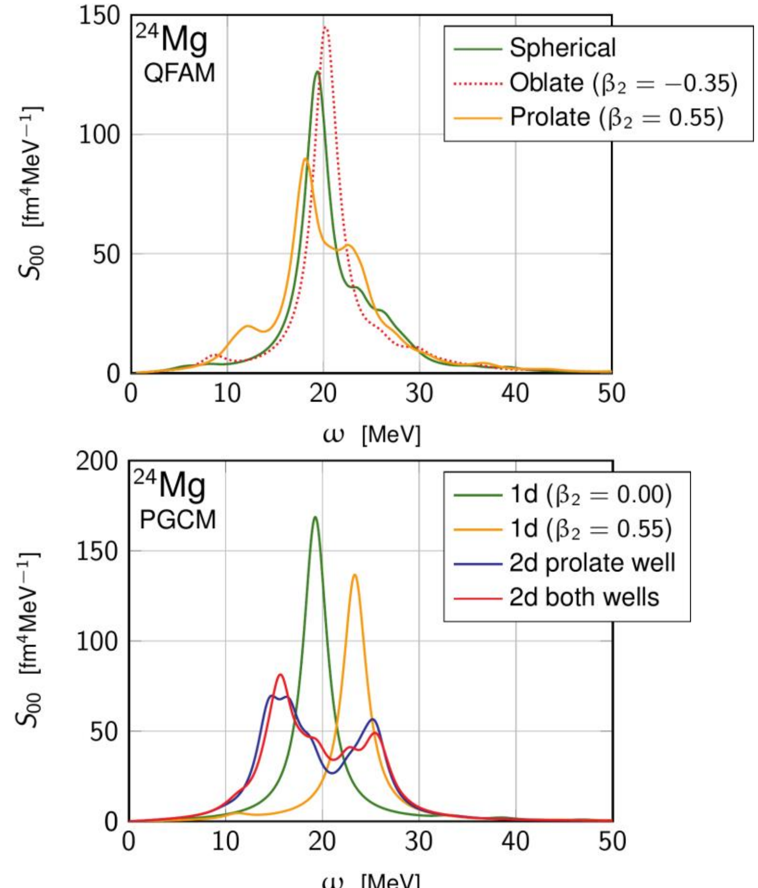

Results

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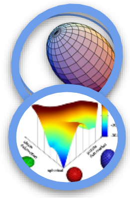
- Important static quadrupole deformation

Deformation effects in ^{24}Mg

Difficulty



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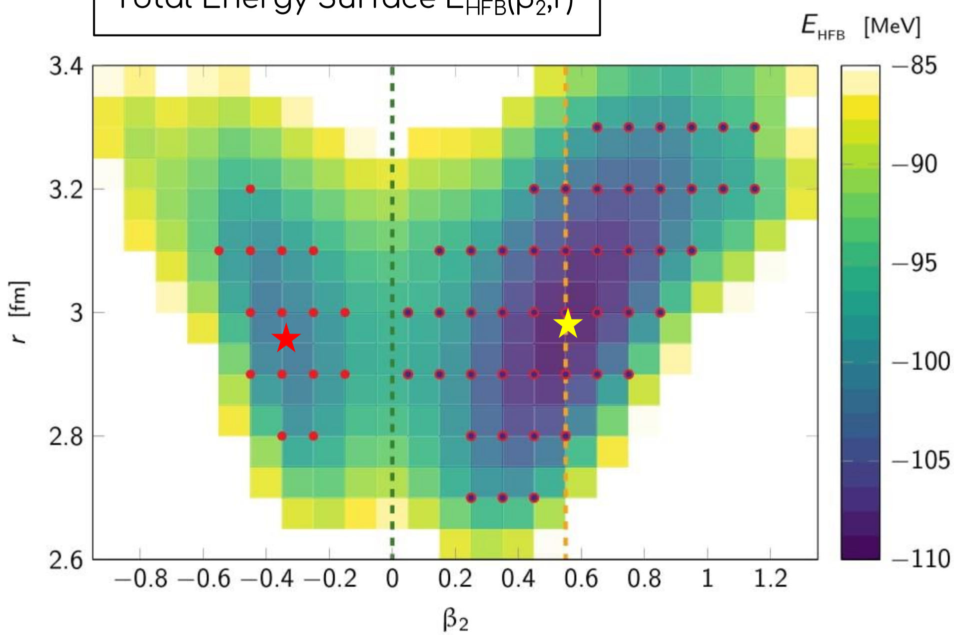

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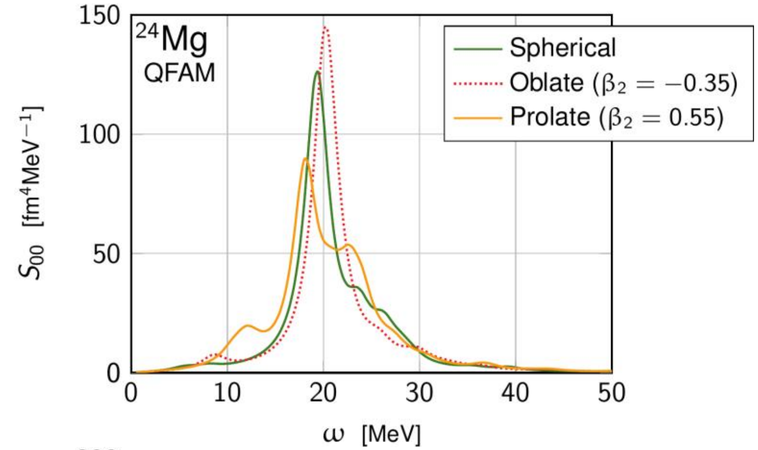
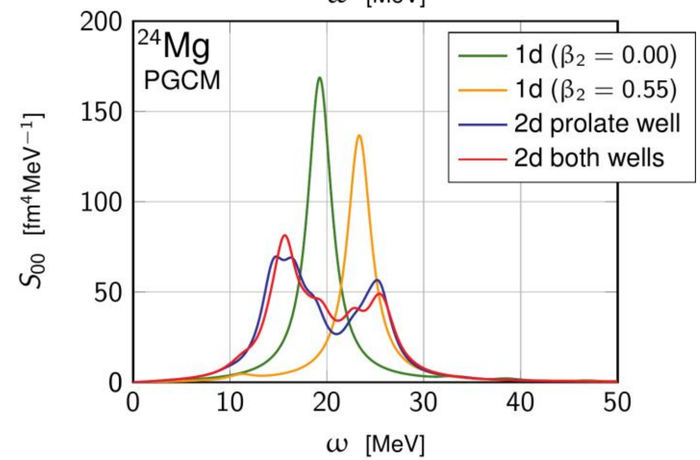


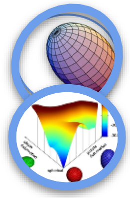


Results

- Dominant prolate minimum
- Important static quadrupole deformation
- Quadrupole fluctuations crucial

Deformation effects in ^{24}Mg

Difficulty



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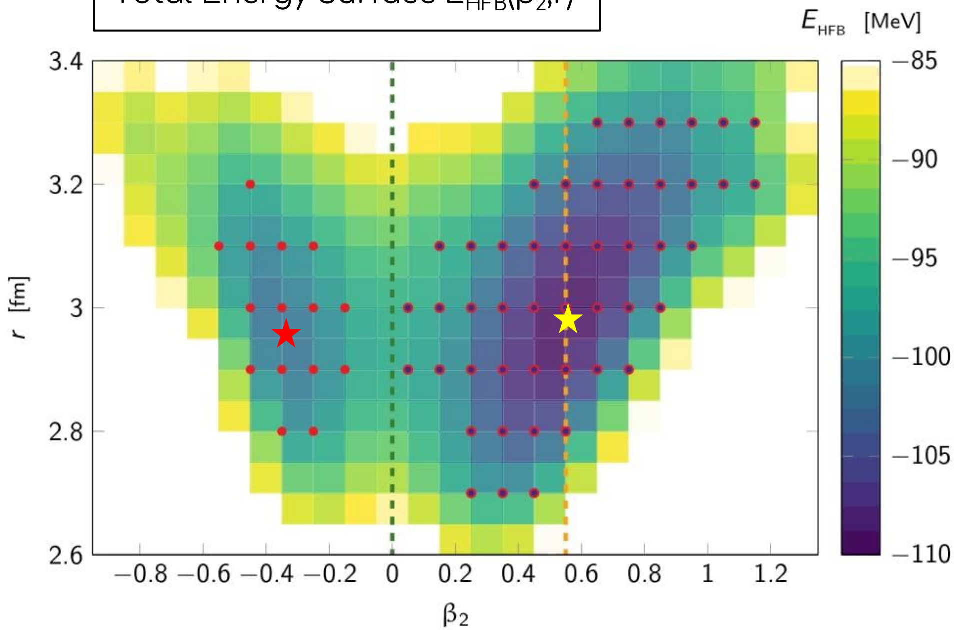

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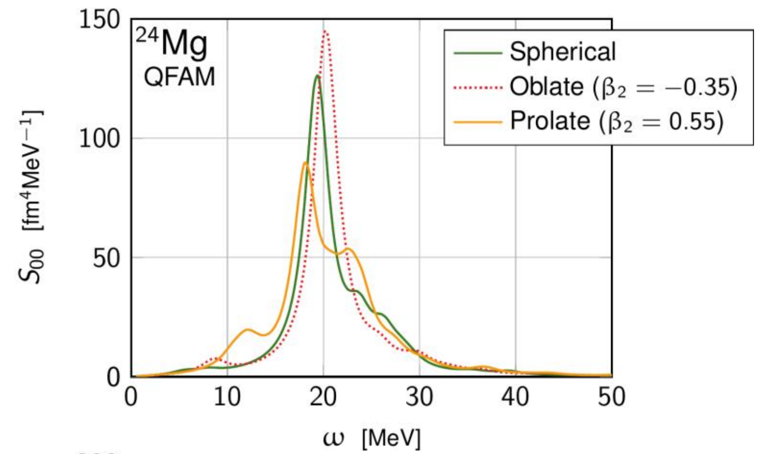

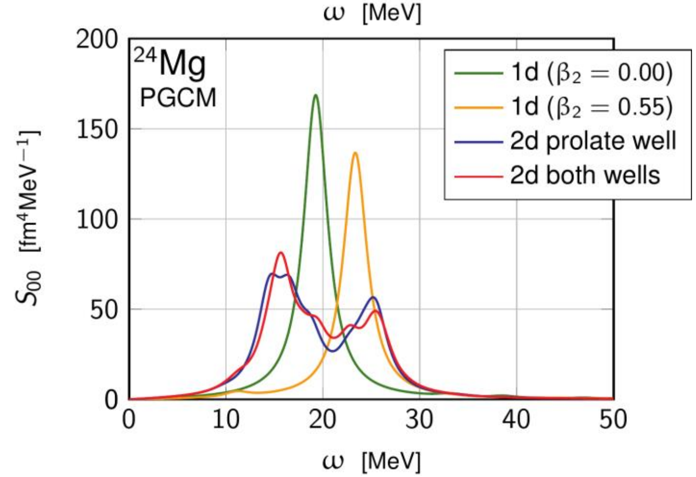

Results

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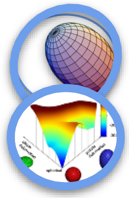
- Quadrupole fluctuations crucial
- No coupling between different wells

Deformation effects in ^{24}Mg

Difficulty



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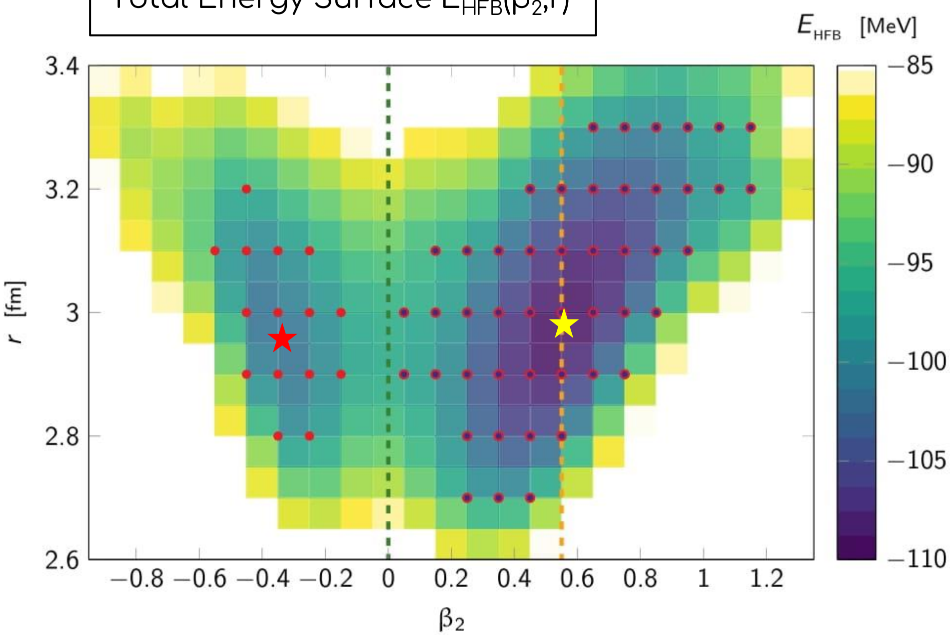

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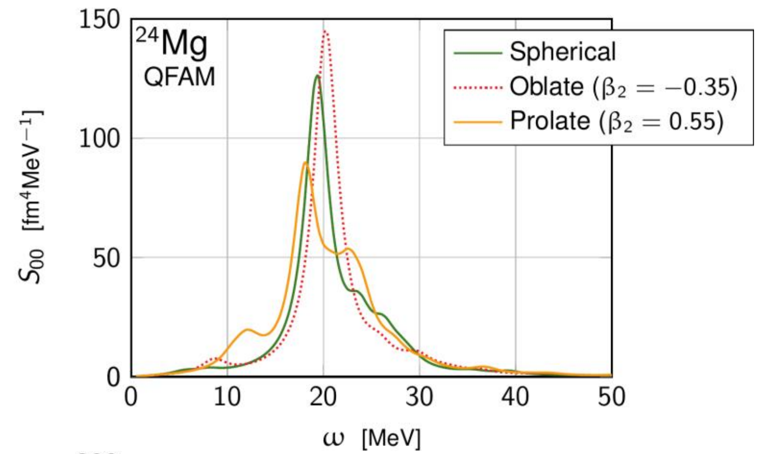

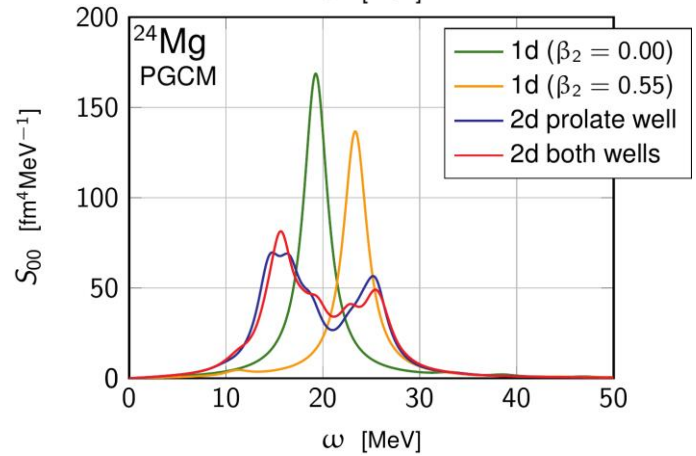

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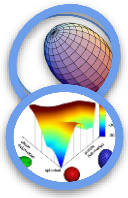
Deformation effects in ^{24}Mg

Difficulty



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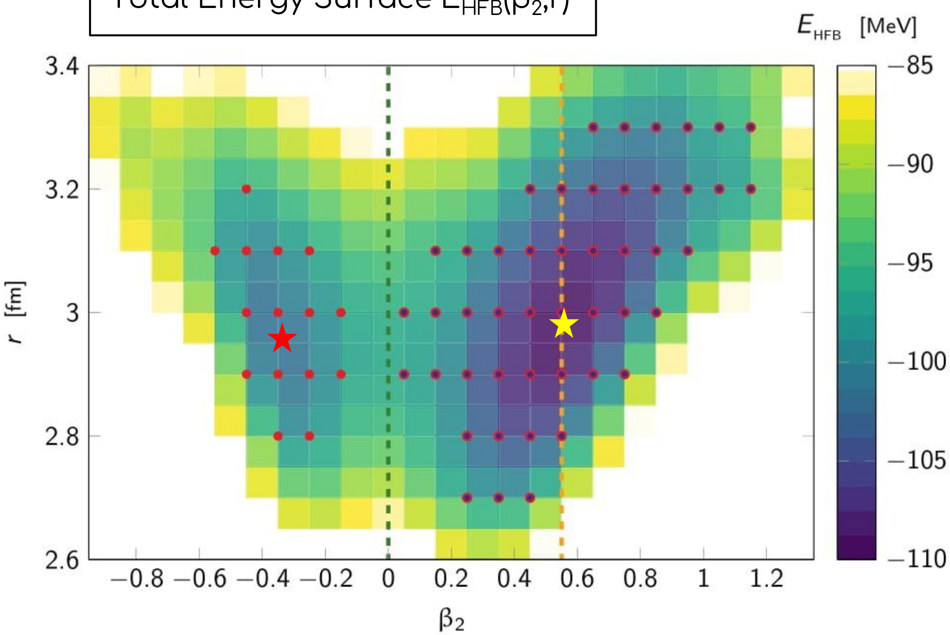

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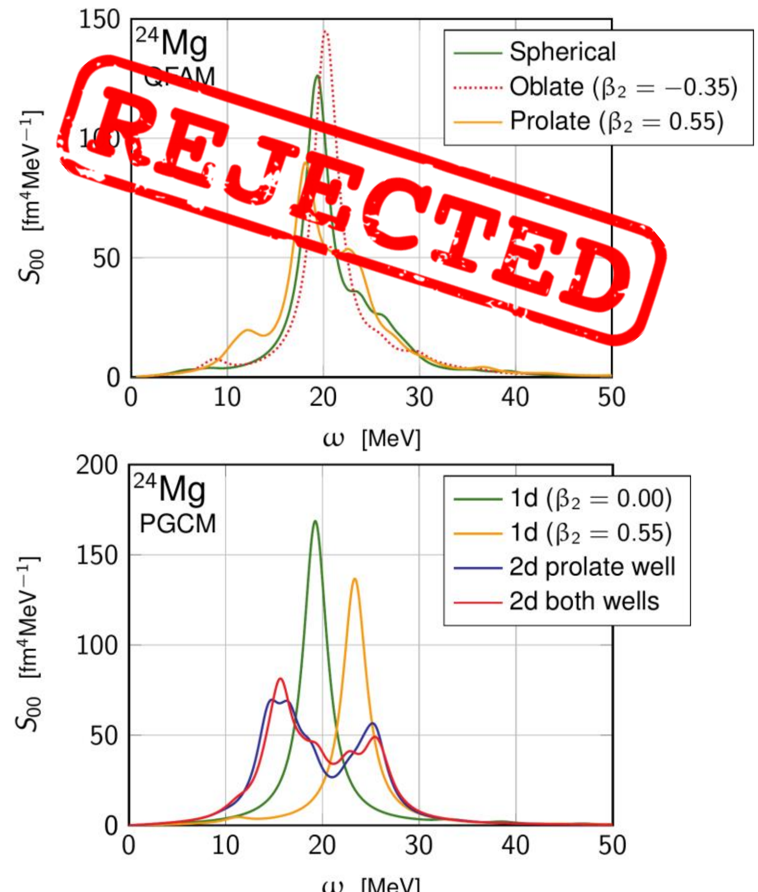

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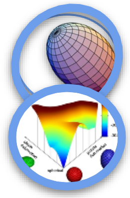

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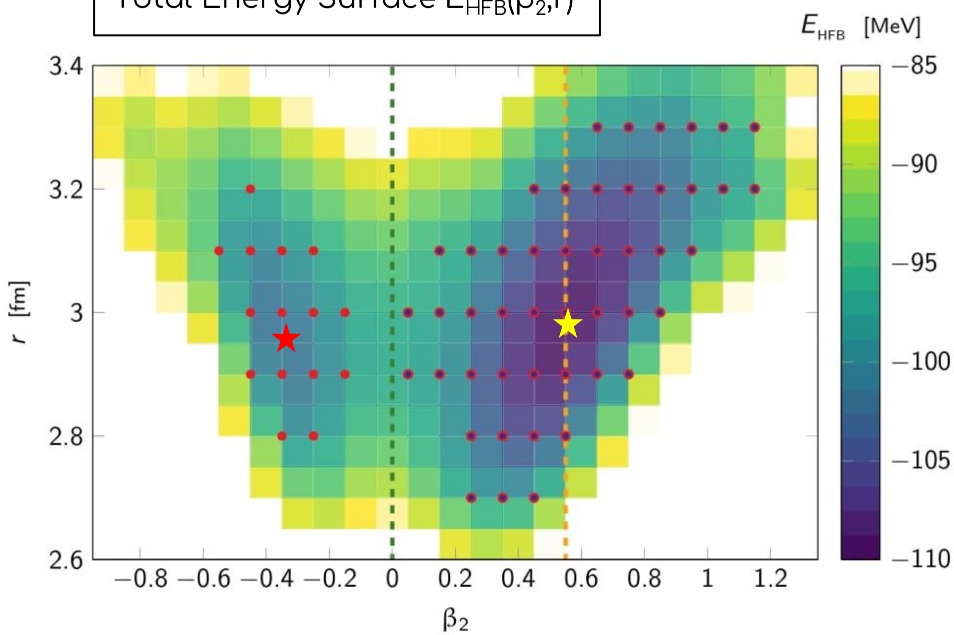
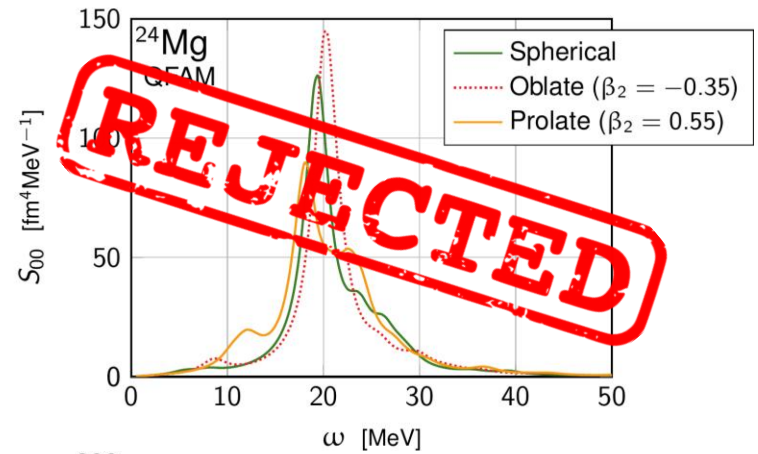
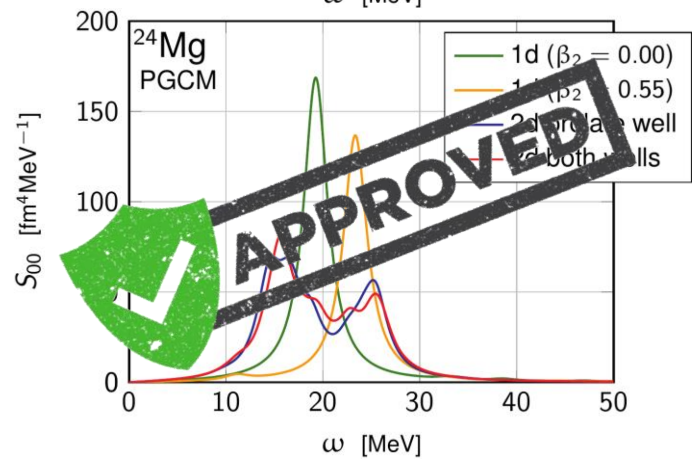


Monopole Strength



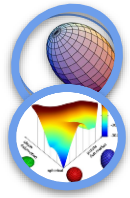


Results

- Dominant prolate minimum
- Important static quadrupole deformation
- Quadrupole fluctuations crucial
- No coupling between different wells
- Important anharmonic effects QRPA unreliable

Deformation effects in ^{24}Mg

Difficulty

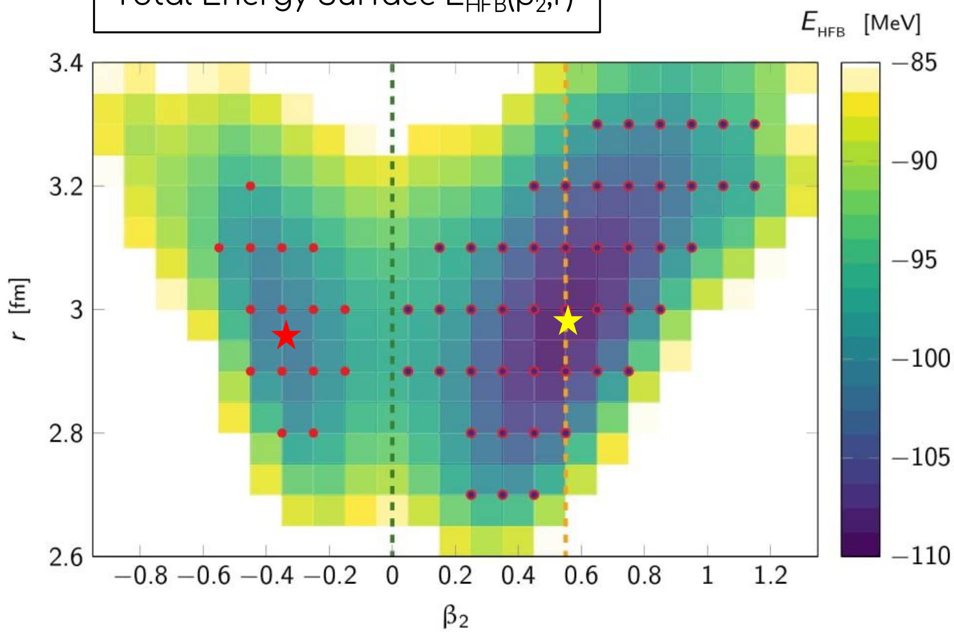


Deformation

Shape coexistence ? [1]

(1) [Dowie et al., 2020]

Total Energy Surface $E_{HFB}(\beta_2, r)$



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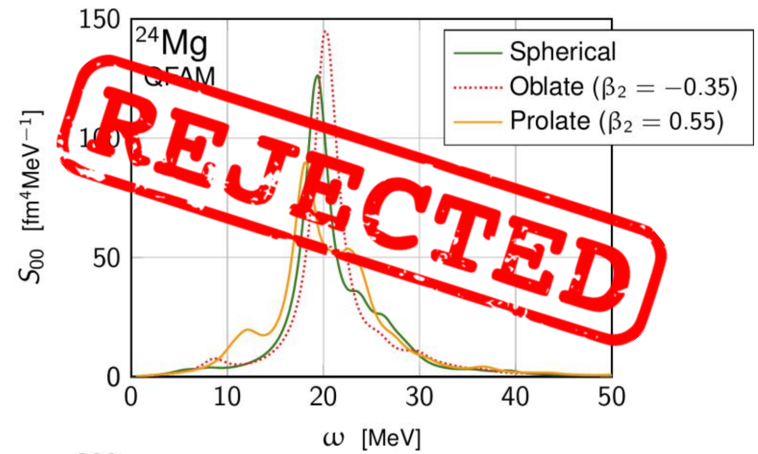

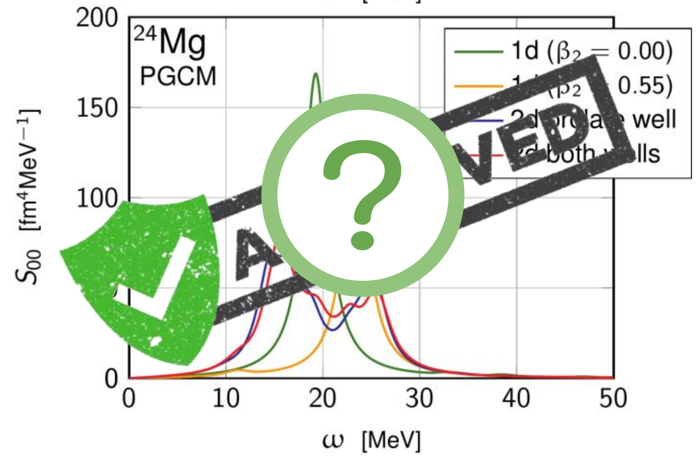

Results

- Dominant prolate minimum
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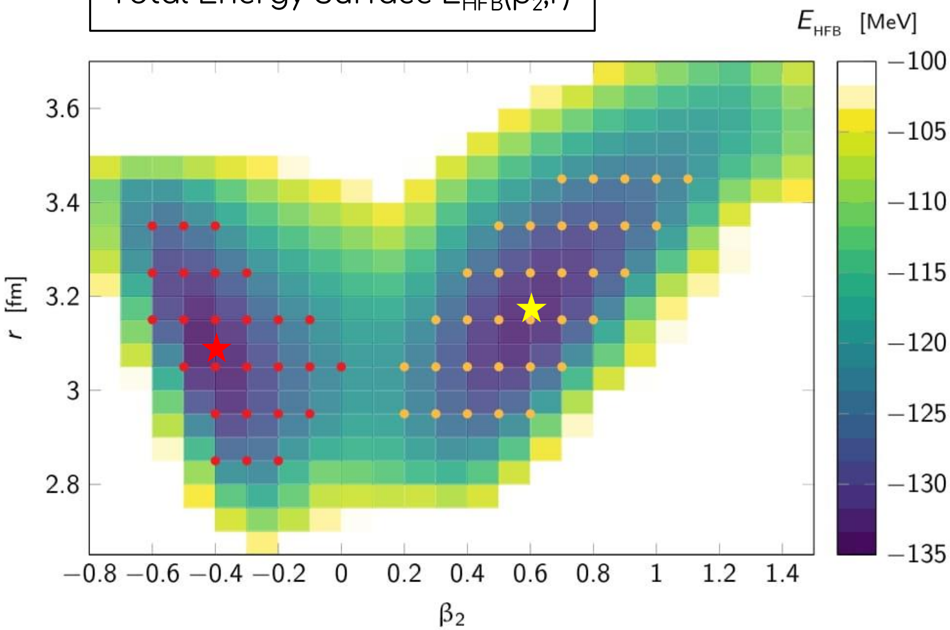
Deformation effects in ^{28}Si

Difficulty

Total Energy Surface $E_{HFB}(\beta_2,r)$



Results

- Two wells clearly separated, oblate dominant

Deformation effects in ^{28}Si

Difficulty

Deformation

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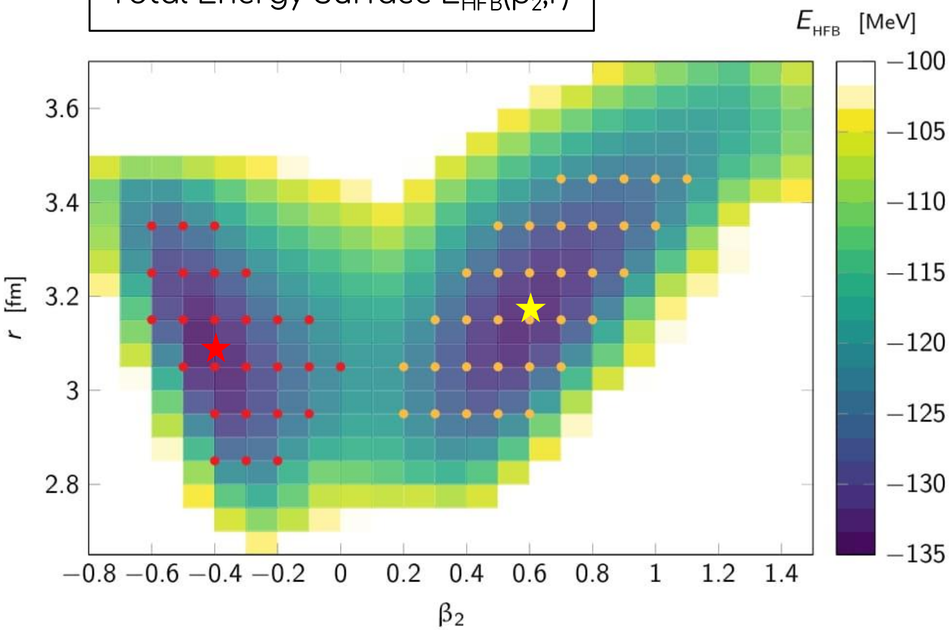

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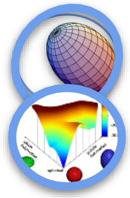

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Shape coexistence ? (1)

(1) [Jenkins et al., 2012]

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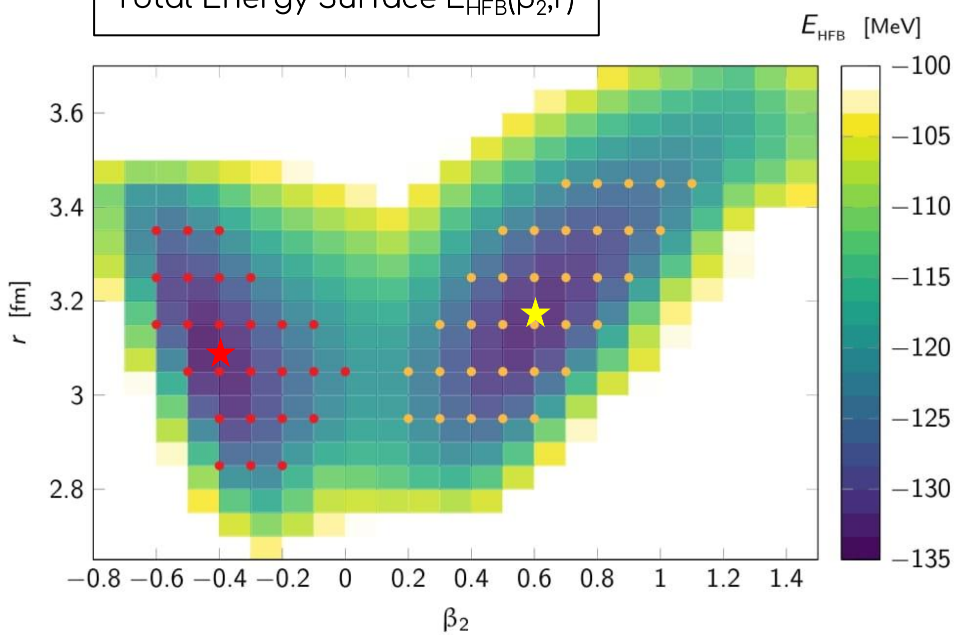

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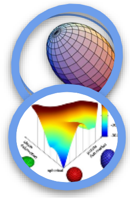

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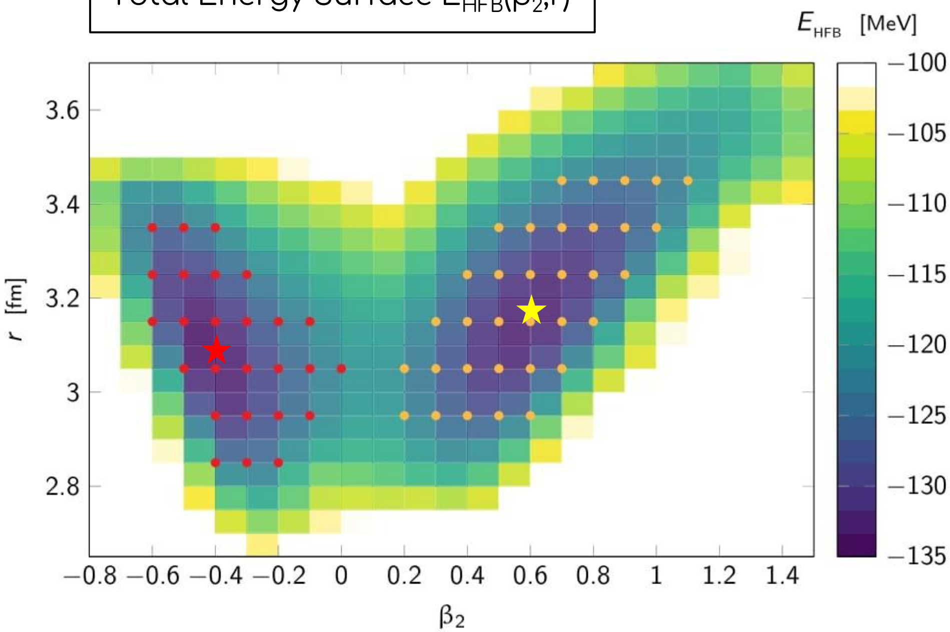

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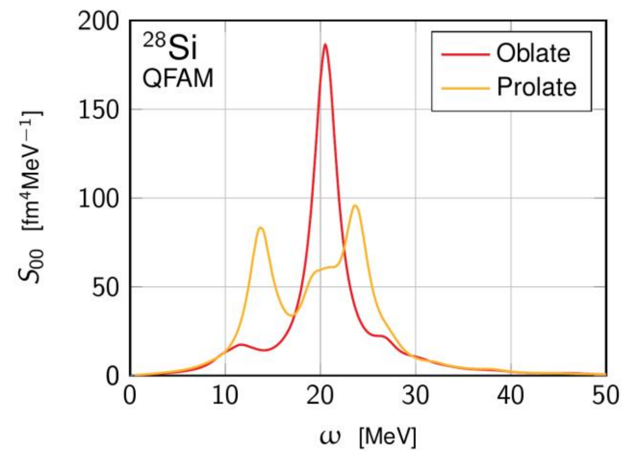
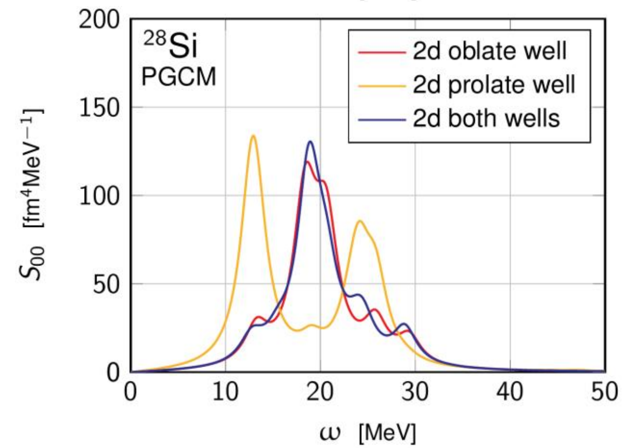


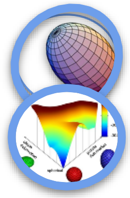


Results

- Two wells clearly separated, oblate dominant
- Qualitatively similar results QFAM/PGCM

Deformation effects in ^{28}Si

Difficulty



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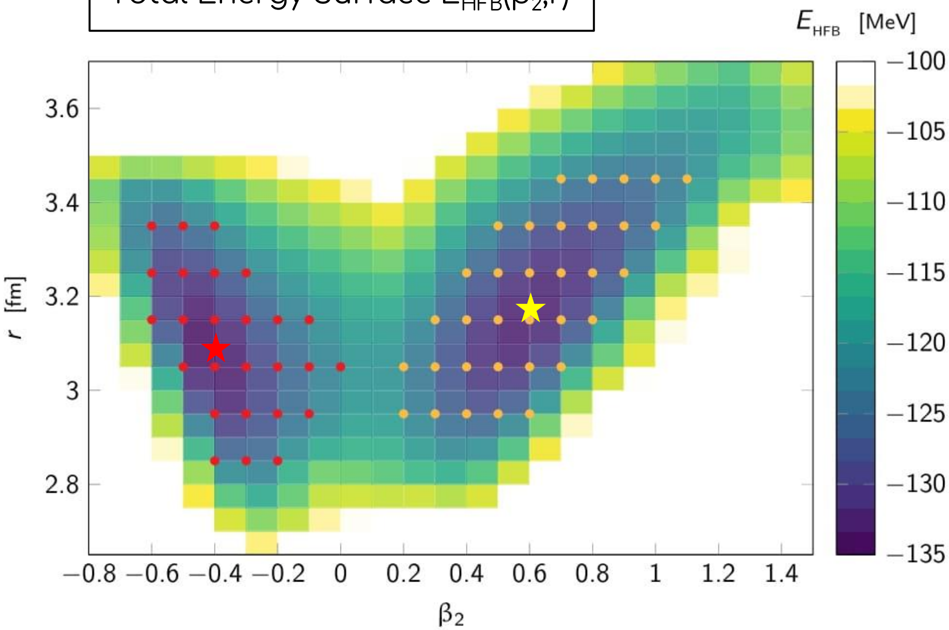
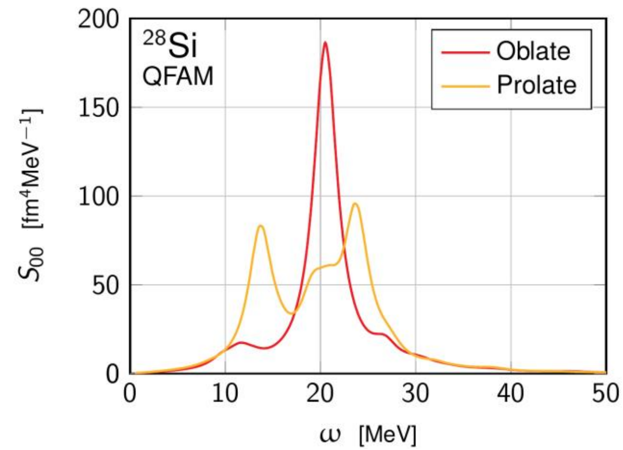
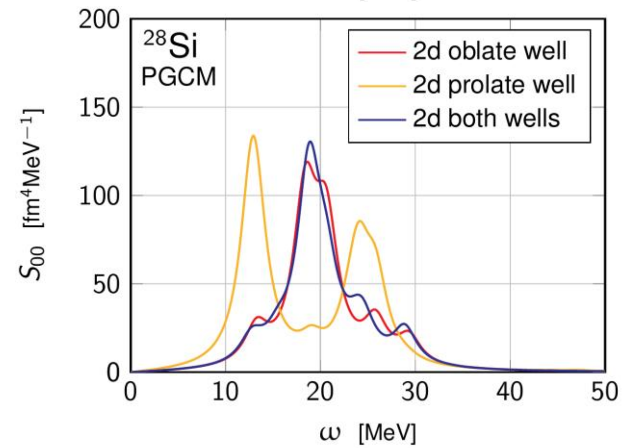


Monopole Strength





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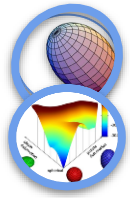

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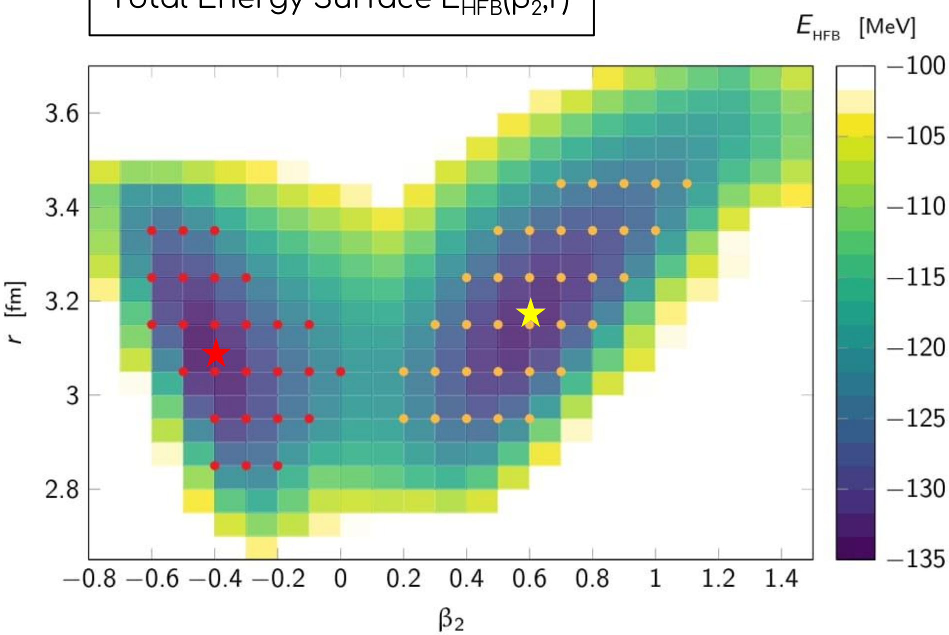

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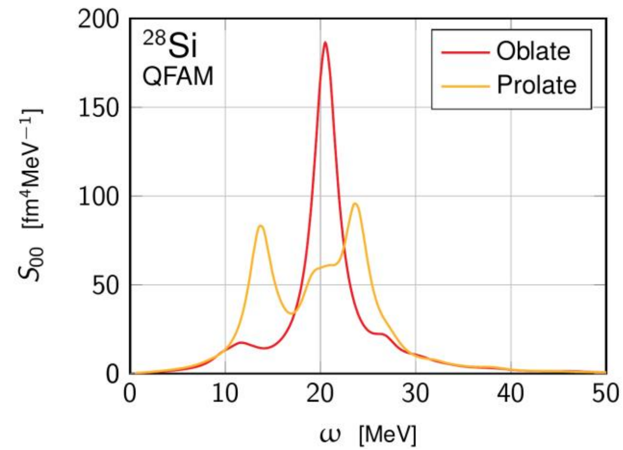
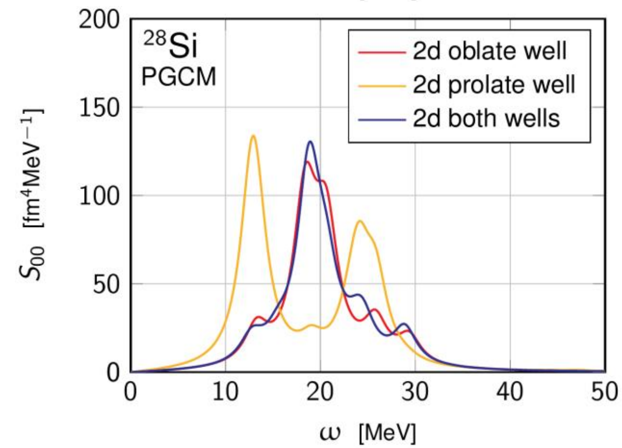


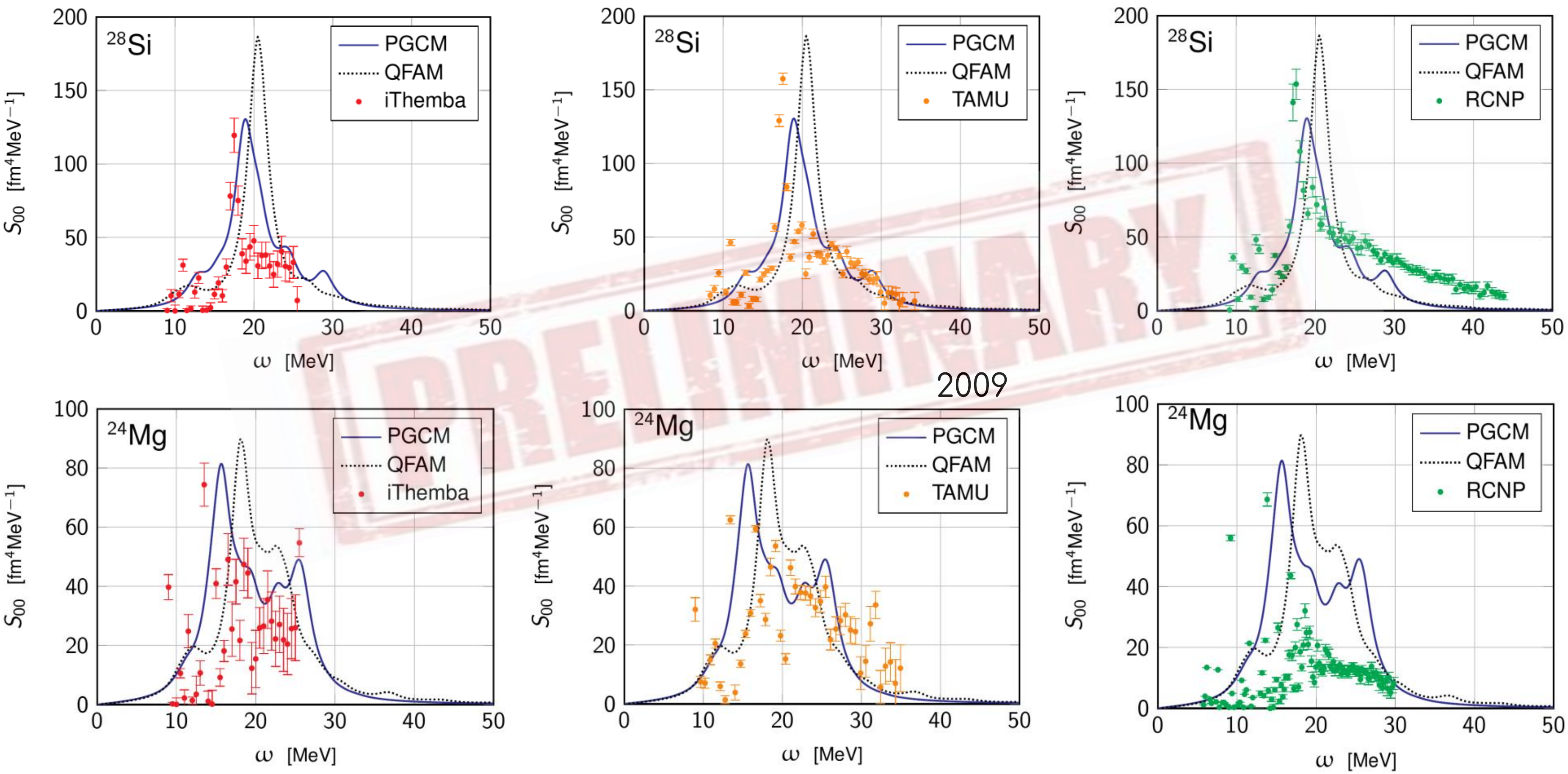


Results

- Two wells clearly separated, oblate dominant
- Qualitatively similar results QFAM/PGCM
- No shape mixing
- Two-peak GMR on the prolate shape isomer ?

Comparison to experiment

iThemba, Bahini 2021 TAMU, Youngblood 2007 RCNP, Kawabata 2013



1. **PGCM superior to QRPA**, i.e. coupling to quadrupole deformation/fluctuations captured
2. Experimental data in doubly open-shell nuclei very useful and promising
3. Data are **not unambiguous**, i.e. better data would be beneficial

Outline

- Introduction
- Formalism
- Preliminary results
- **Conclusions**

Conclusions and Perspectives

First **ab-initio** systematic description of GMR

Choose physics according to selected coordinates

No limitation on the nucleus choice

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First ab-initio systematic description of GMR

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No limitation on the nucleus choice

Plan of the complete study

- ☐ Static quadrupolar deformation
- ☐ Coupling to quadrupolar vibrations
- ☐ Shape isomers
- ☐ Theoretical comparison of moment computation
- ☐ Hamiltonian uncertainty through different chiral EFT orders
- ☐ Superfluidity (Oxygen isotopic chains, pairing variations)
- ☐ Bubble structure (^{34}Si and ^{36}S)
- ☐ Nuclei of current experimental interest (^{68}Ni and ^{70}Ni) [MSU, AT-TPC]

Conclusions and Perspectives

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- [x] Static quadrupolar deformation
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And more if you have suggestions !

Thanks for the attention

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