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

Methods, uses and new preliminary results

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Vittorio Somà

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Advances on giant nuclear monopole excitations and applications to multi-messenger Astrophysics
ECT* Trento

Outline

- Introduction
- Formalism
- Preliminary results
- Conclusions

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  - Ab-initio methods for ground- and excited states
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Input Hamiltonian

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Many-body solution

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Global philosophy

The approximate solution must be systematically improvable and approach the exact solution in a well-defined limit.

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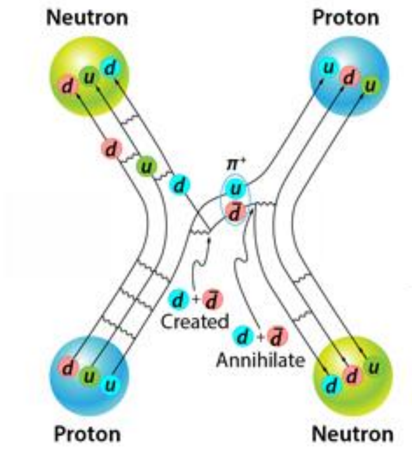

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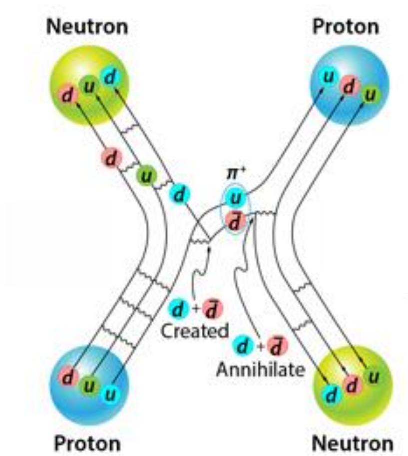
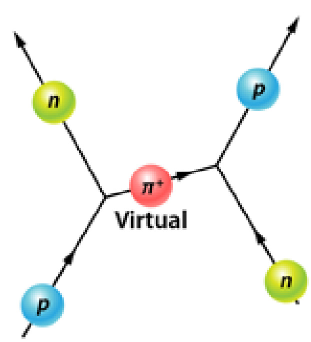


Nuclear forces



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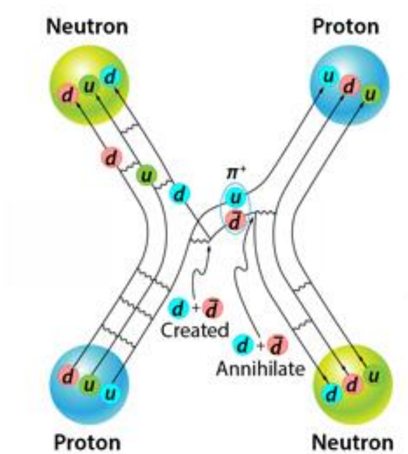

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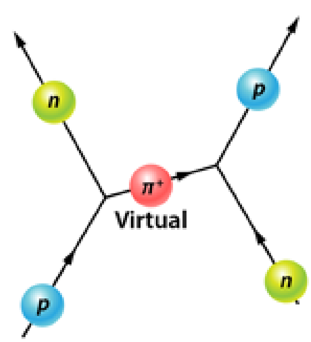

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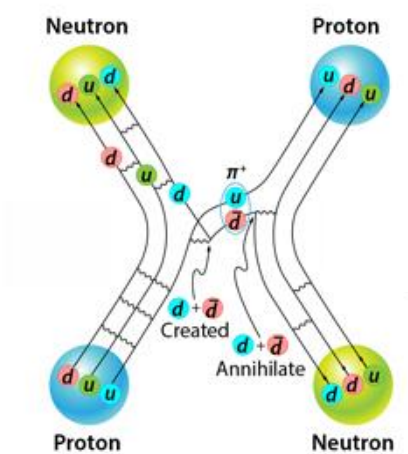

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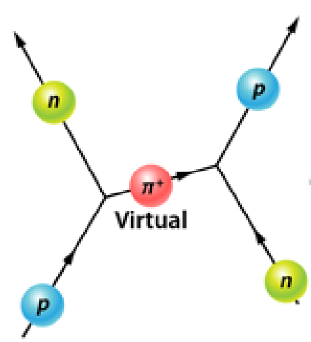

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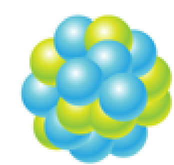

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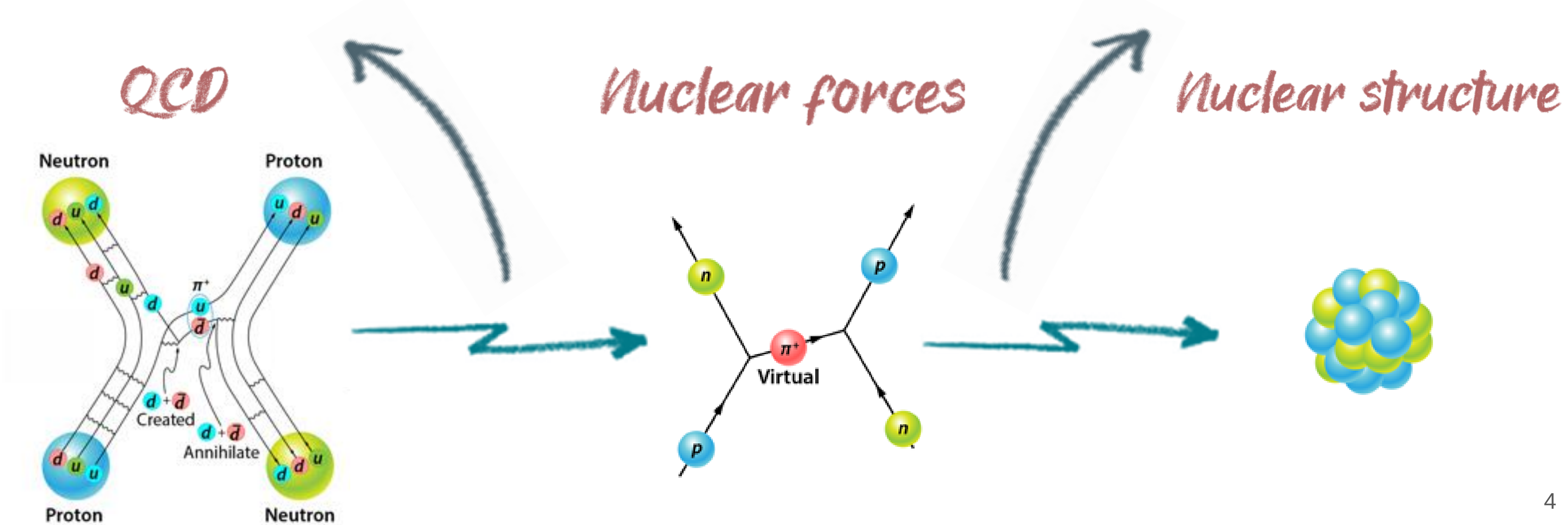
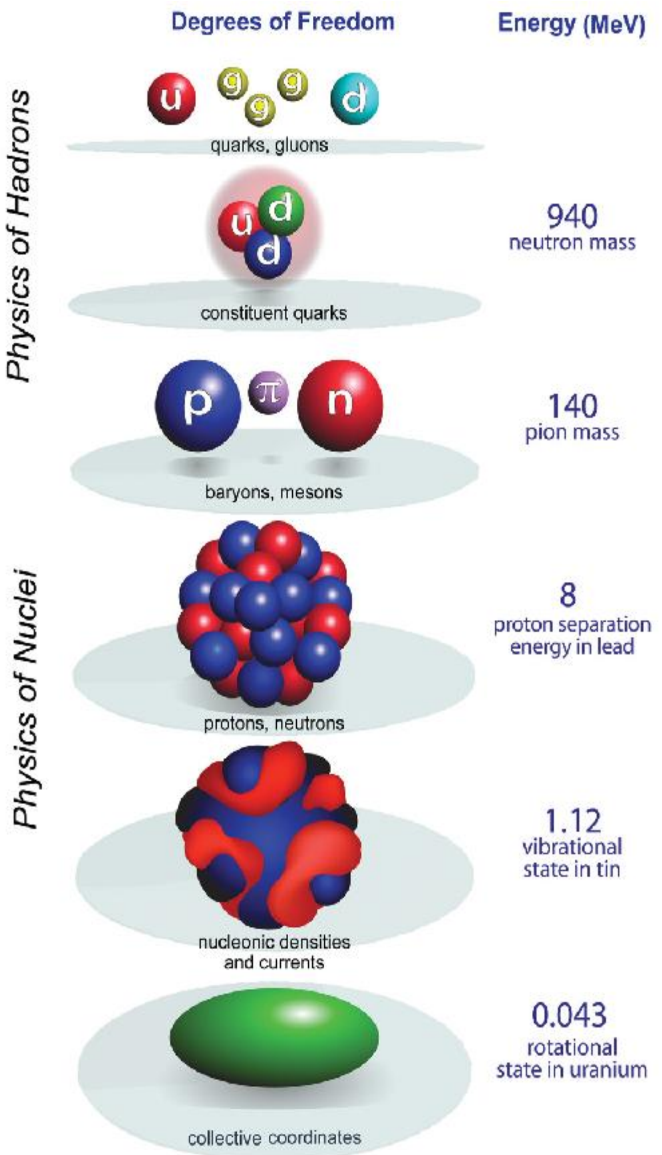


The tower of EFTs



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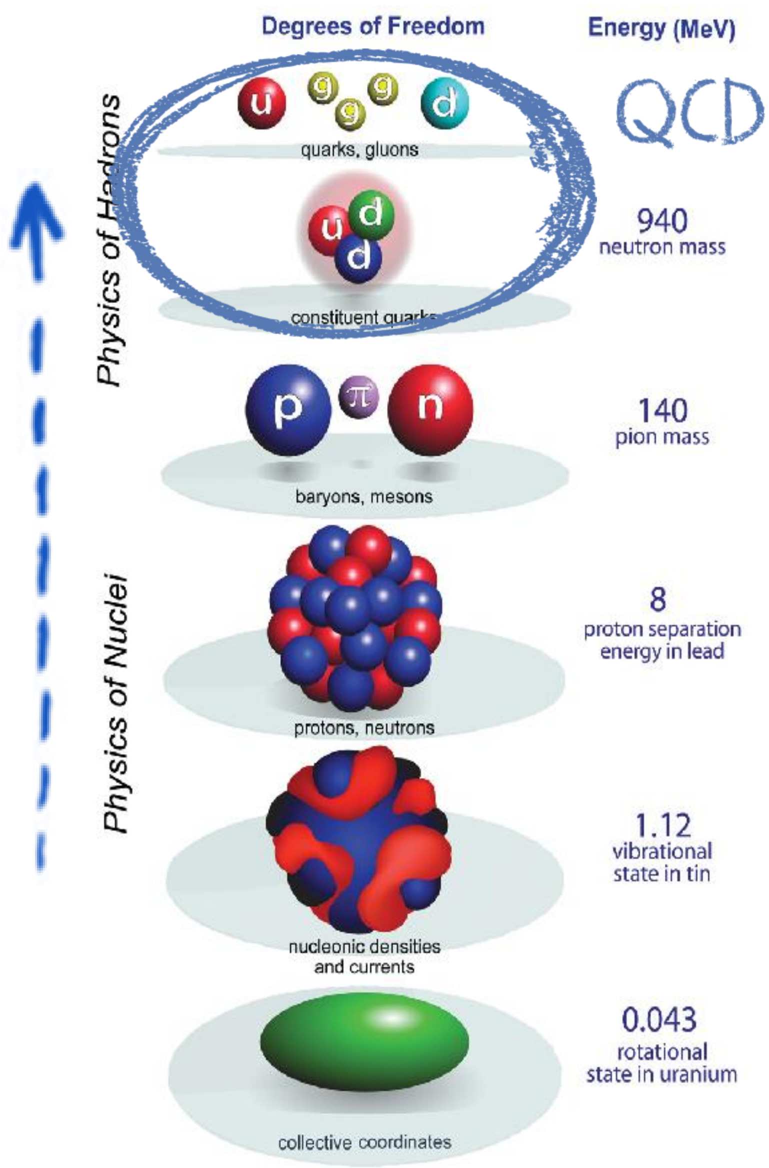

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- More elementary description
- Complexity in terms of elementary DOF
- Lattice QCD

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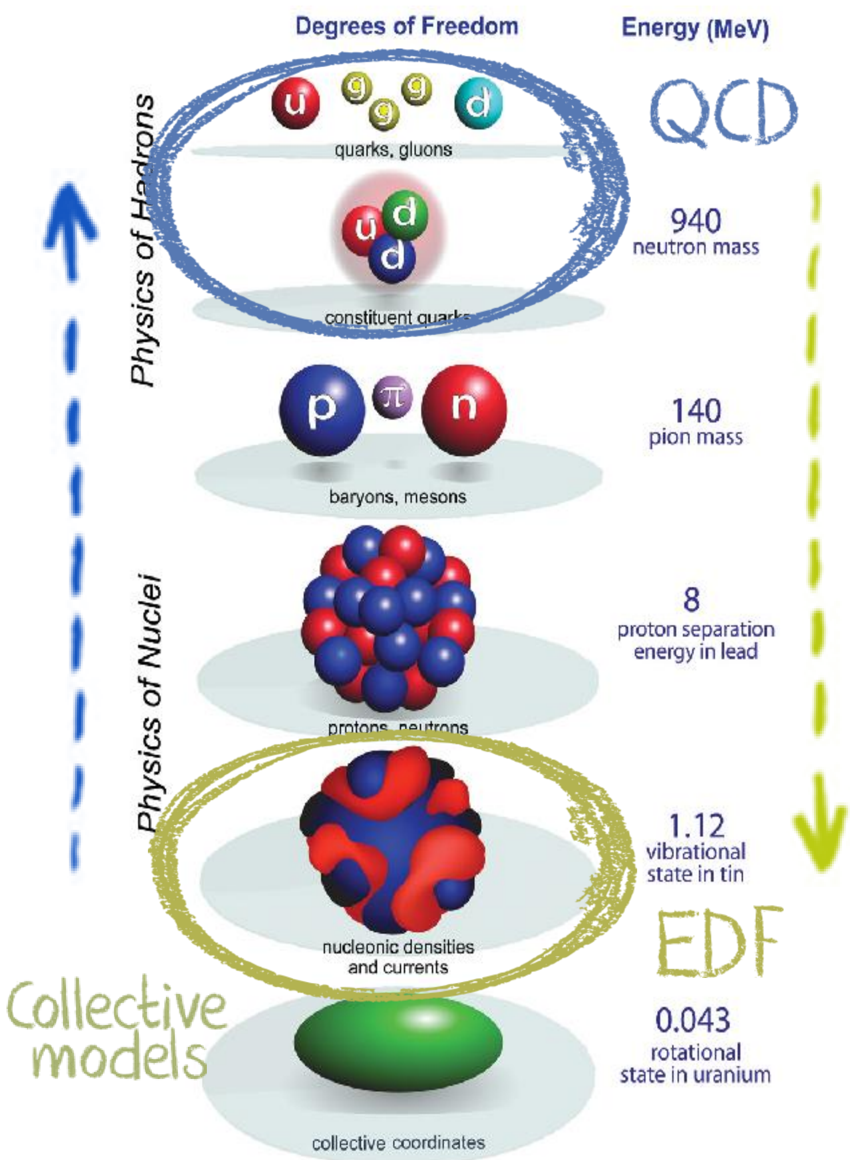

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- Collective picture
- Phenomena from effective description
- Energy Density Functional
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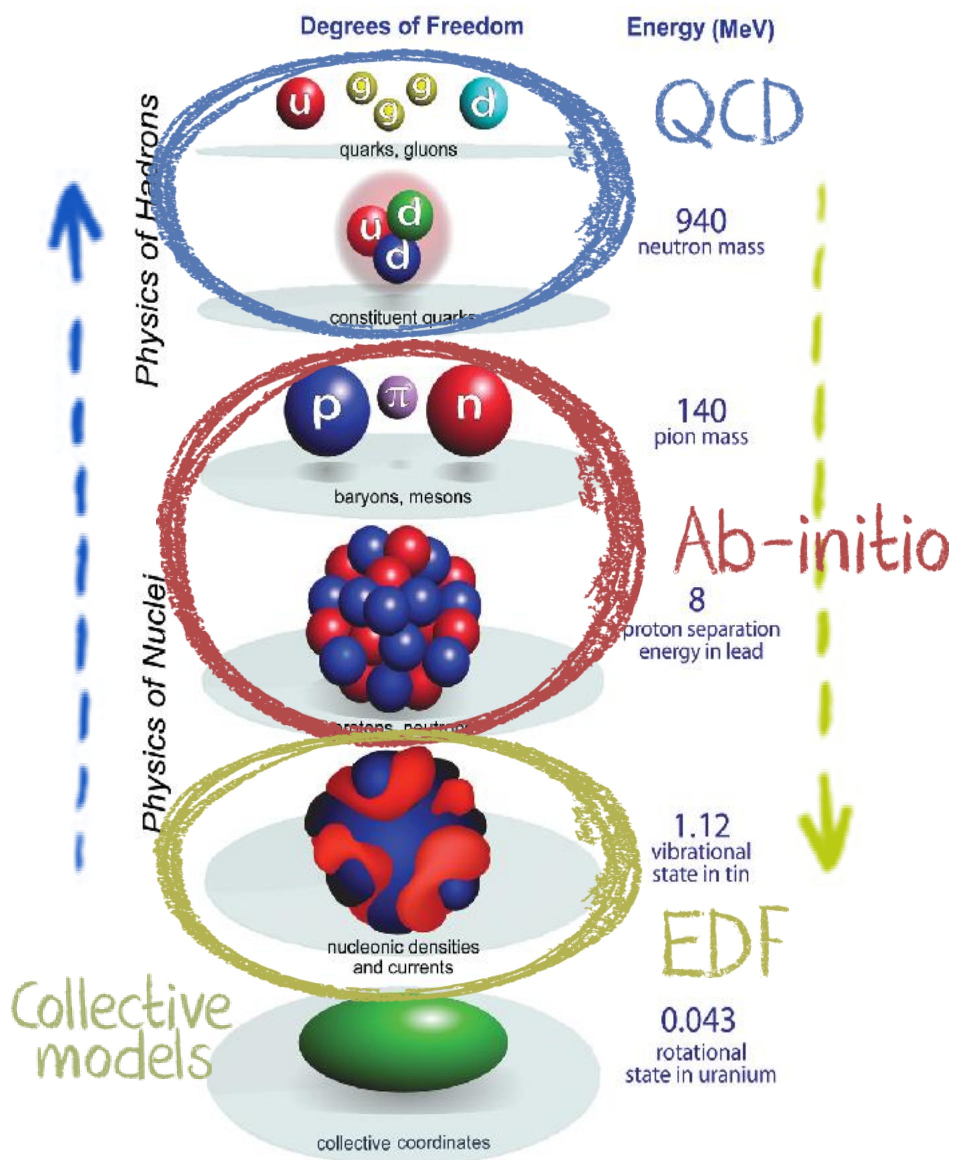

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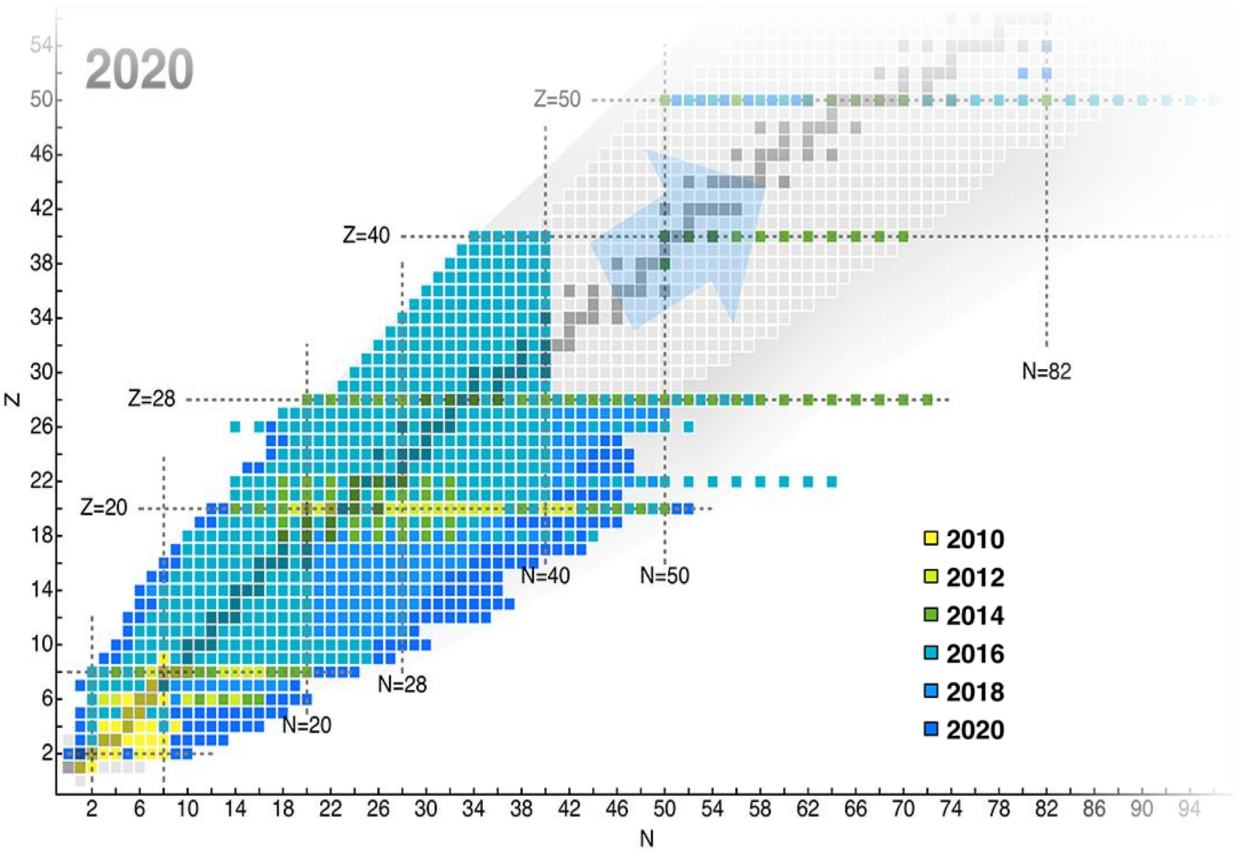
X-EFT

- Structure-less Protons and Neutrons
- All nucleons are active
- Systematically improvable
- LEC from data (or simulations)
- Up to A-body forces

The ab-initio timeline



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- Factorial scaling
- Monte-Carlo methods and NCSM
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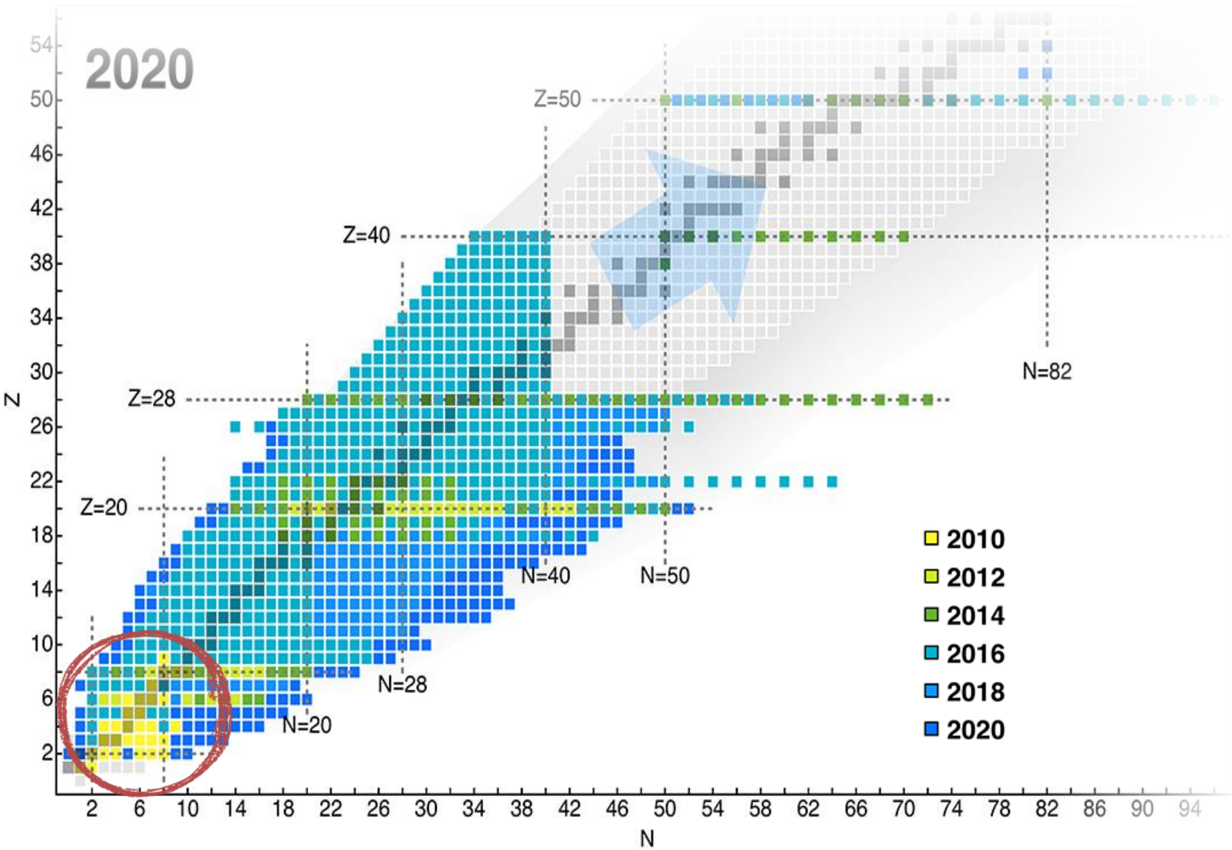

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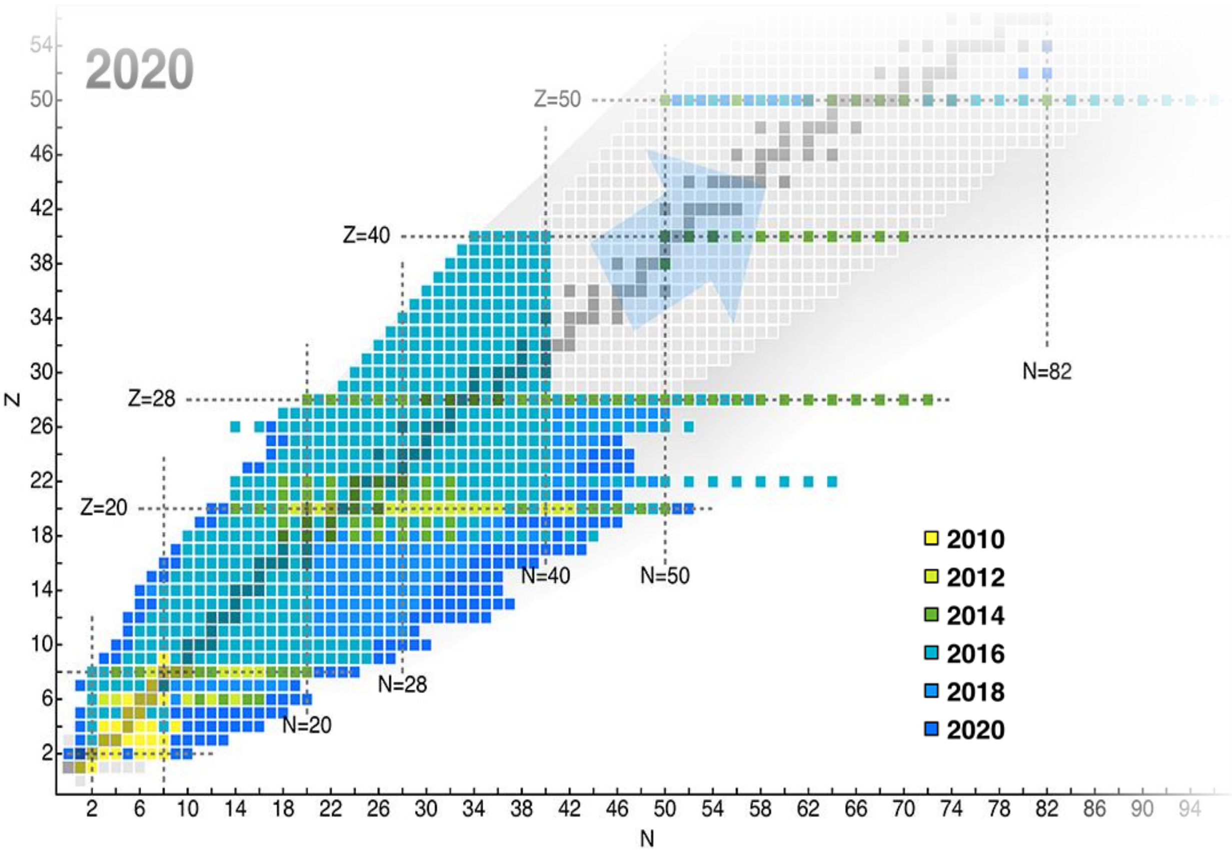

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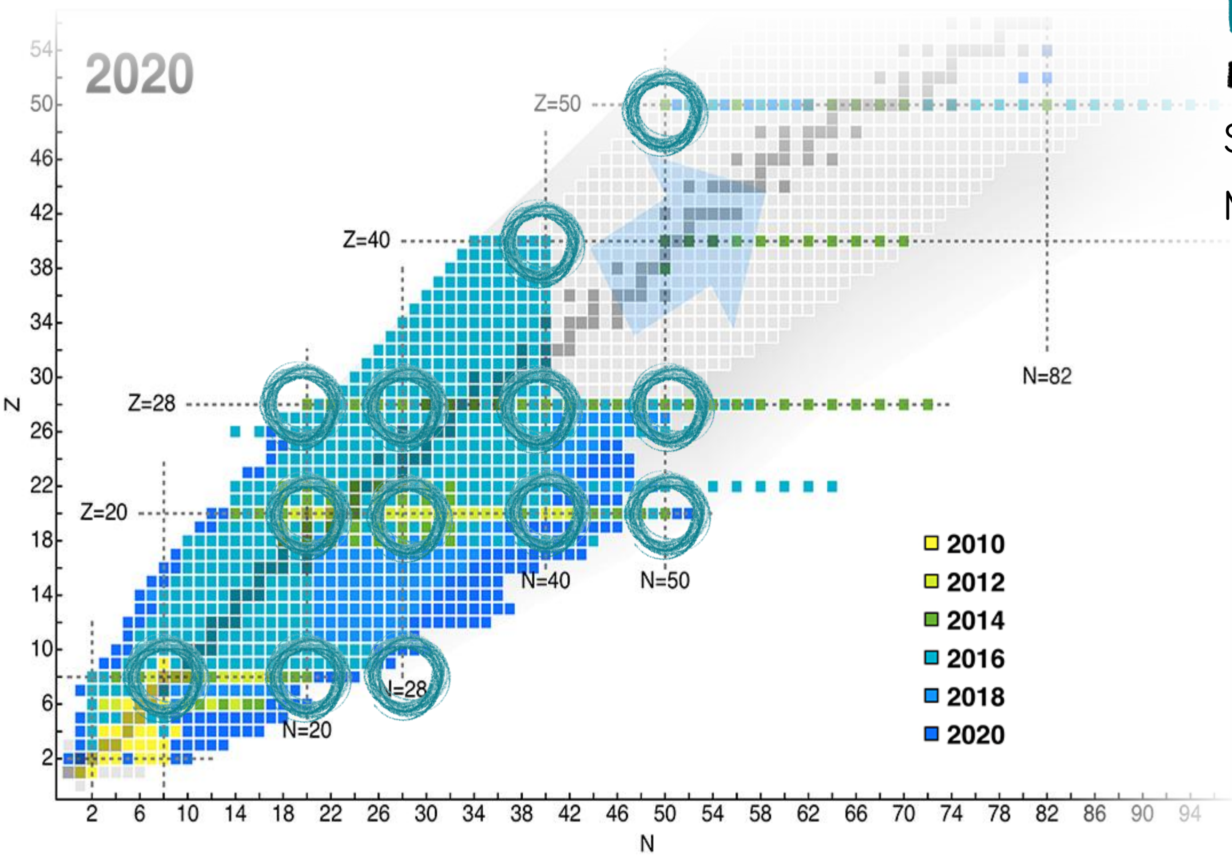

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From 2005

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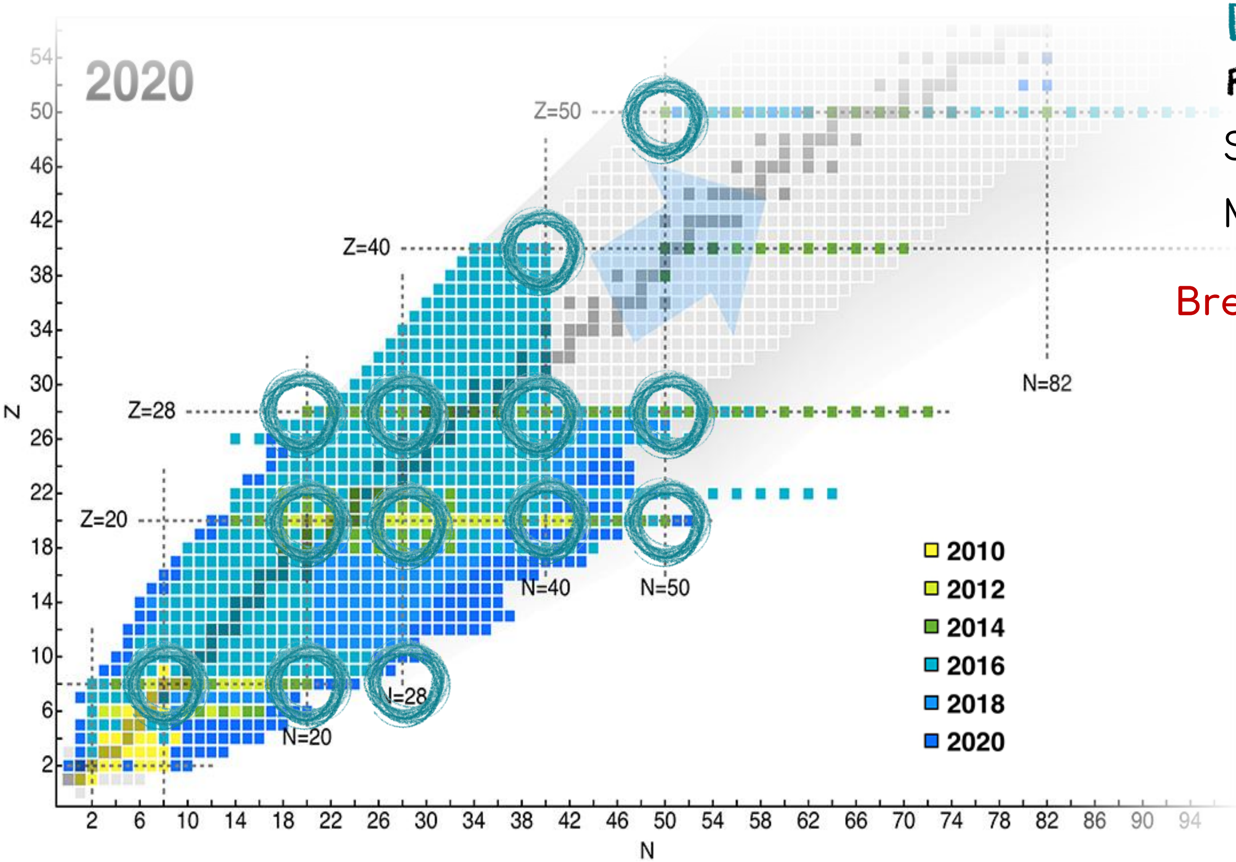

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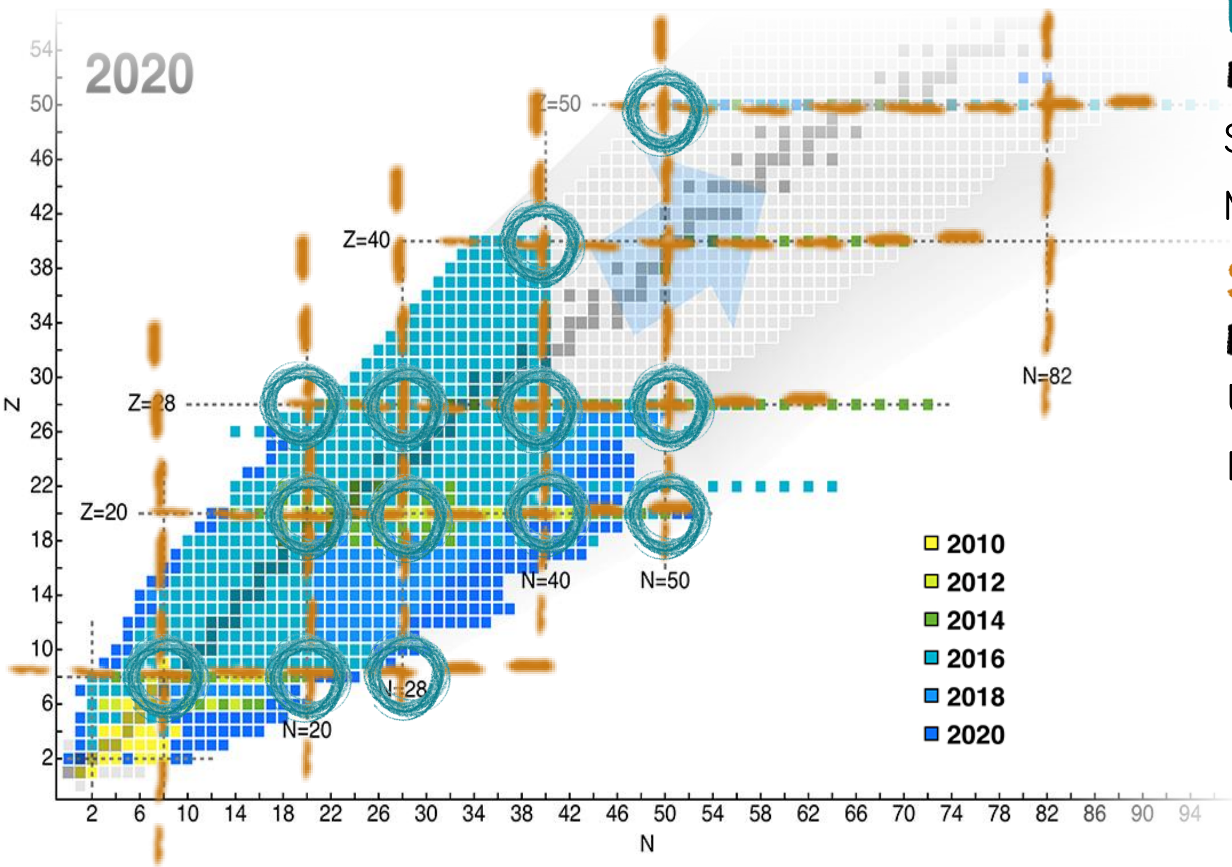

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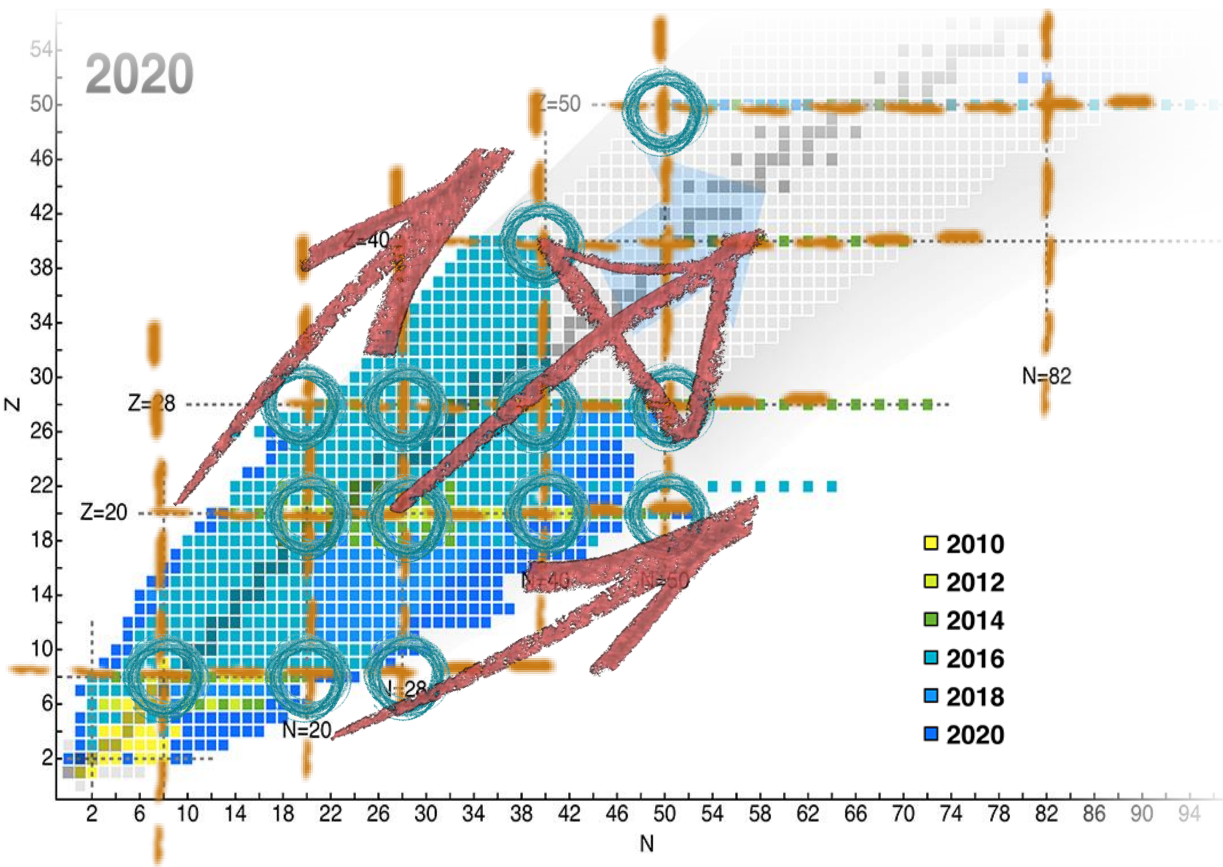

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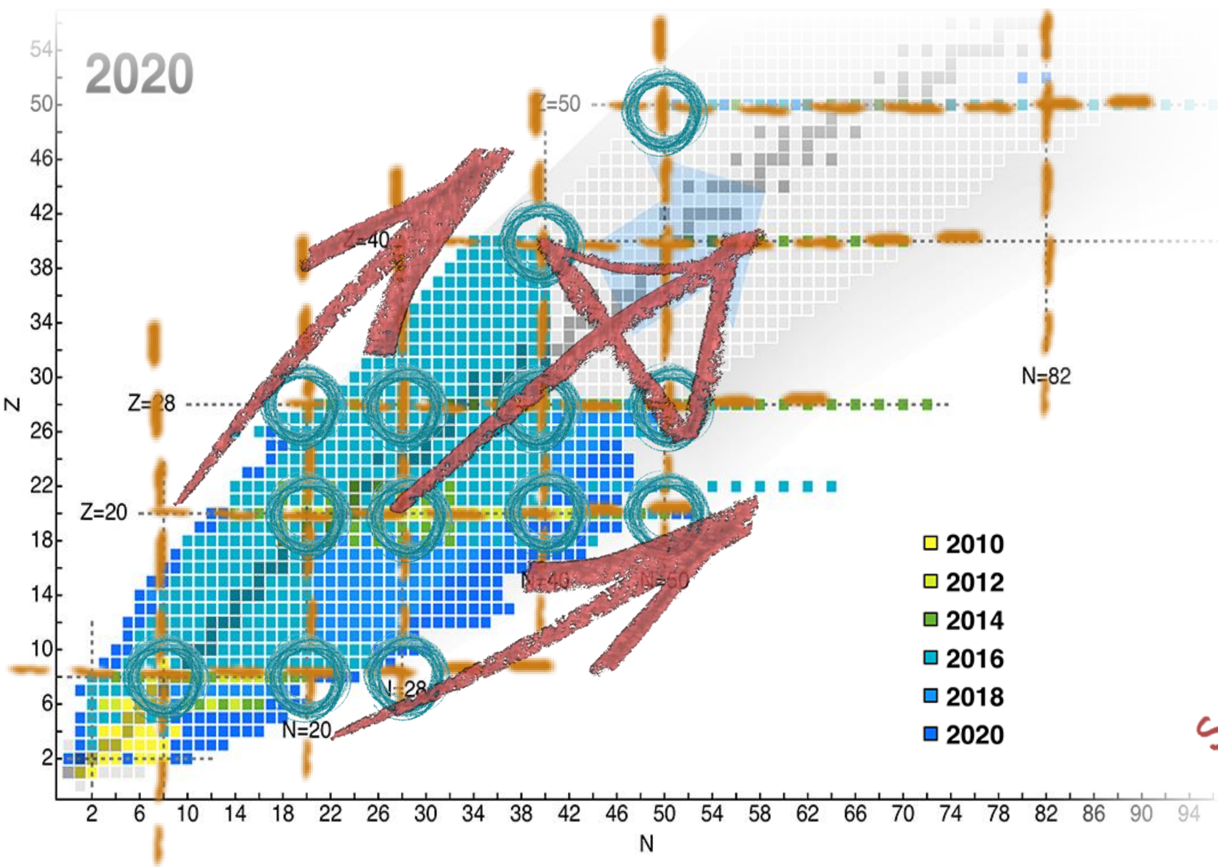

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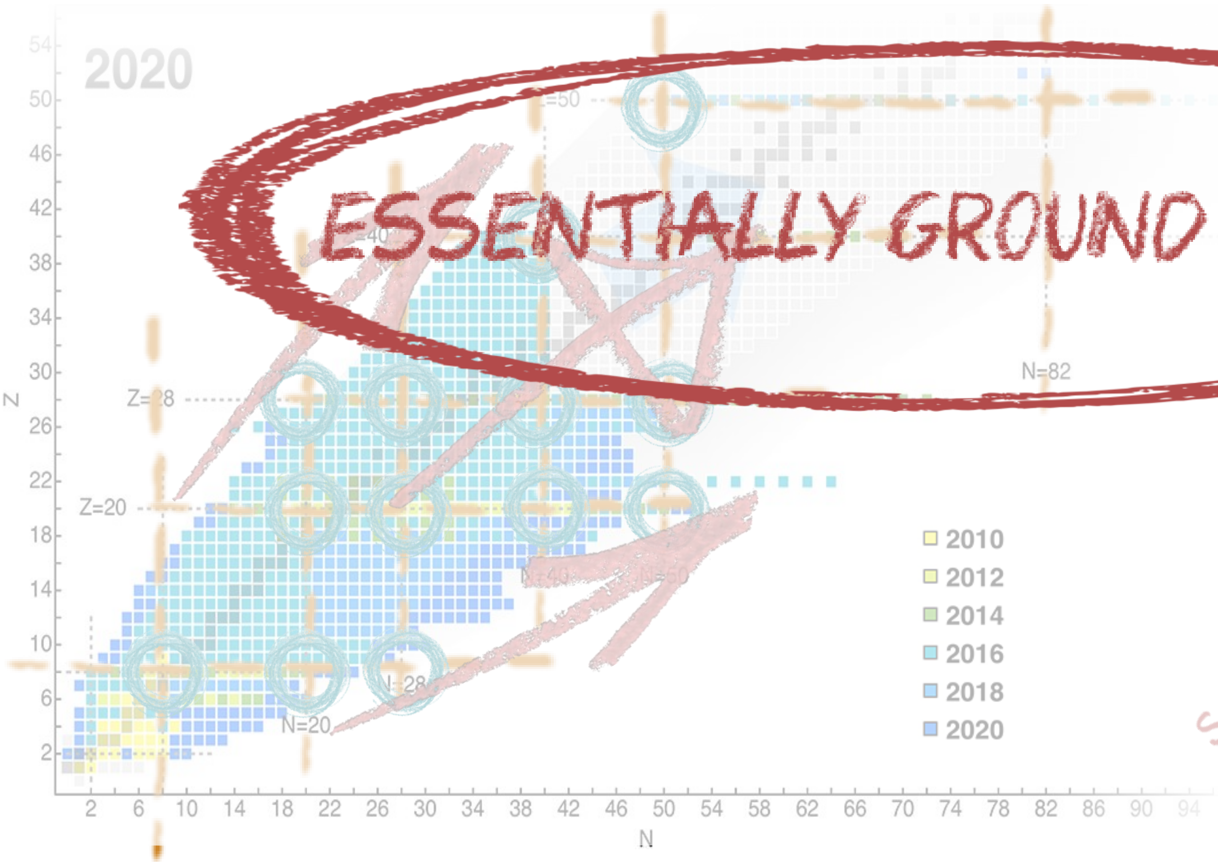

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ESSENTIALLY GROUND STATE

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EOM-Like techniques

- Ground-state relies on previous calculations
- Excited states from the action of linear operators
- Similar to the Equation of Motion
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(EOM-CC)

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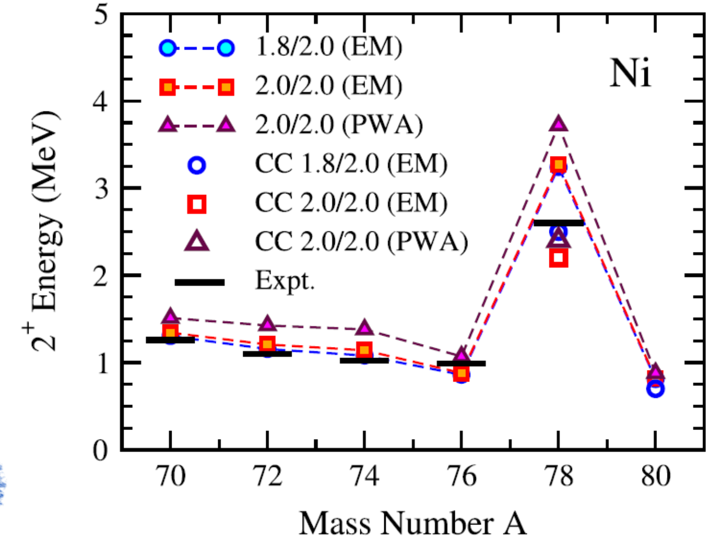
[From H. Hergert, Frontiers in Physics, 2020]



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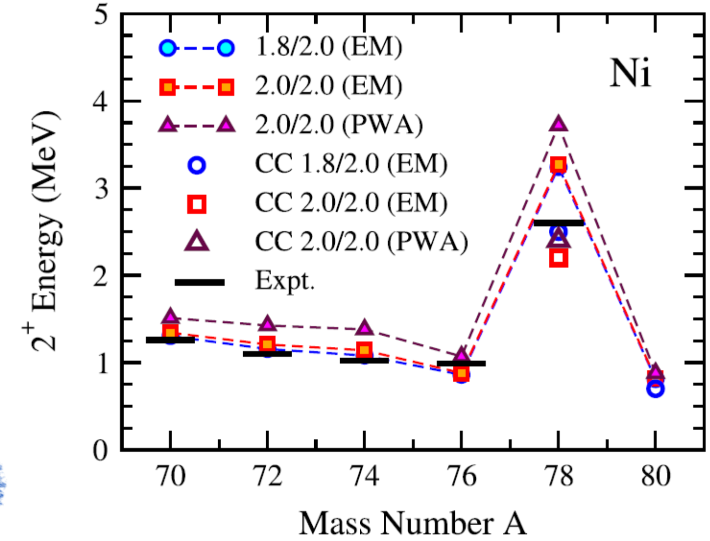

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Wave operator acting separately on excited states

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(PGCM-PT)

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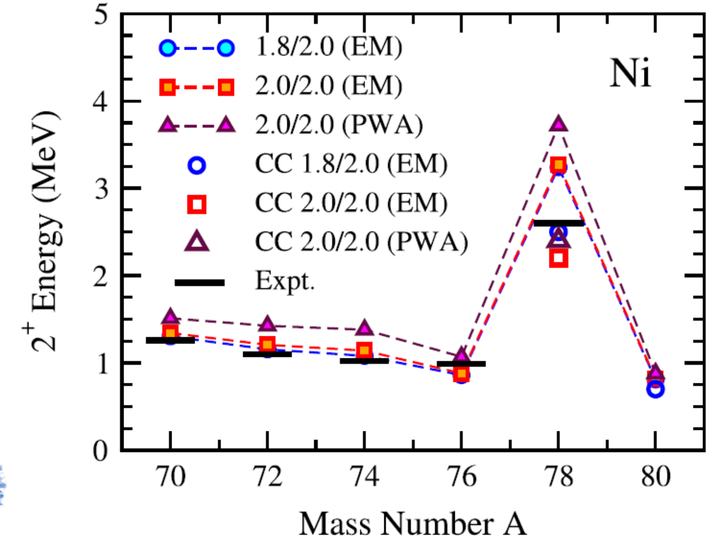

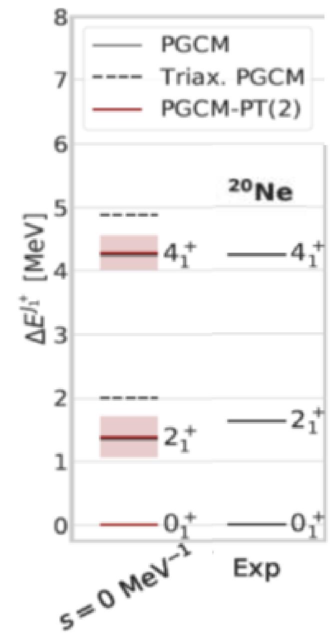

[Frosini et al. , EPJA, 2022]

Collective excitations

Lorentz integral transform

- Reduction to bound-state problem
- Numerical inversion issues
- The response should consist of 1/2 broad peaks

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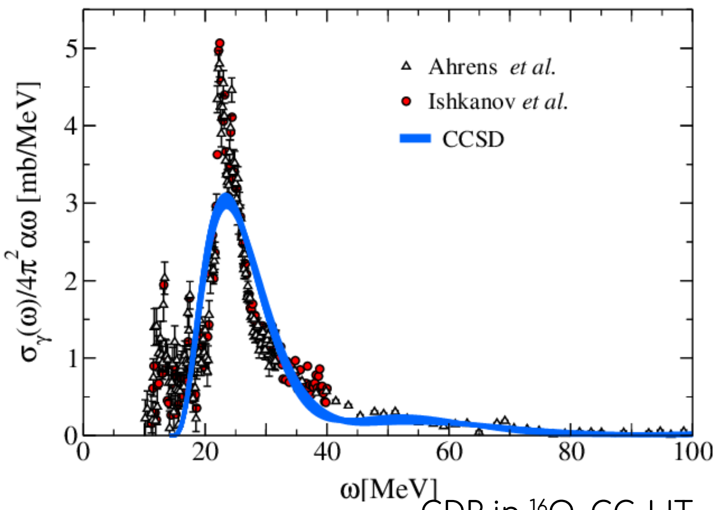

GDR in ^{16}O, CC-LIT

[Bacca et al., PRL 2013]

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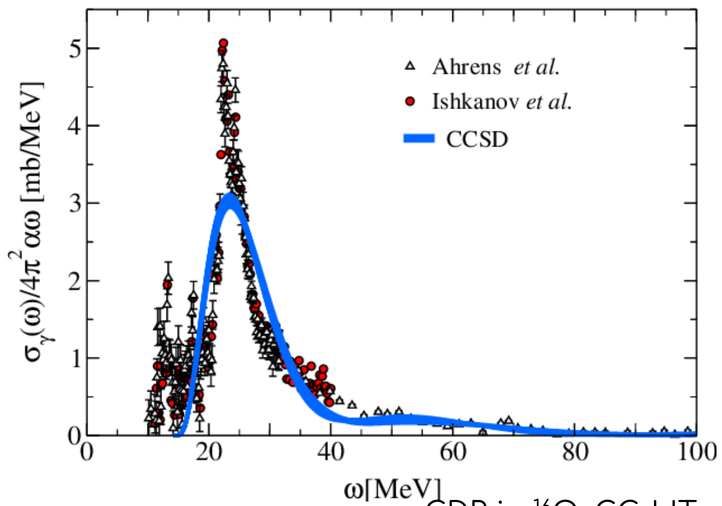

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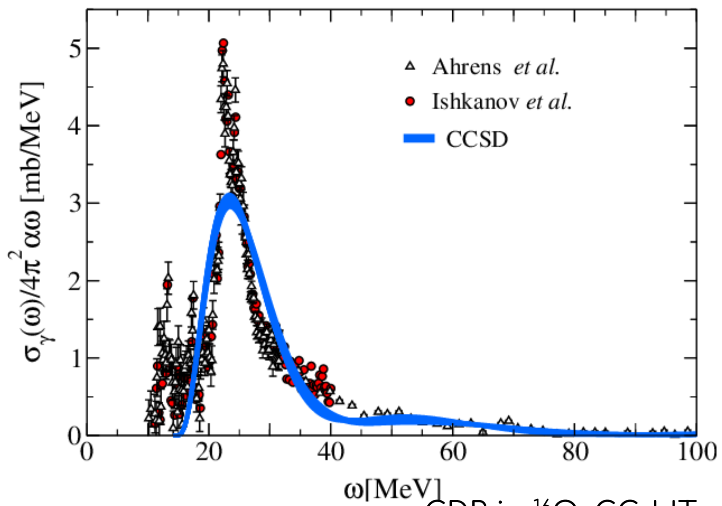

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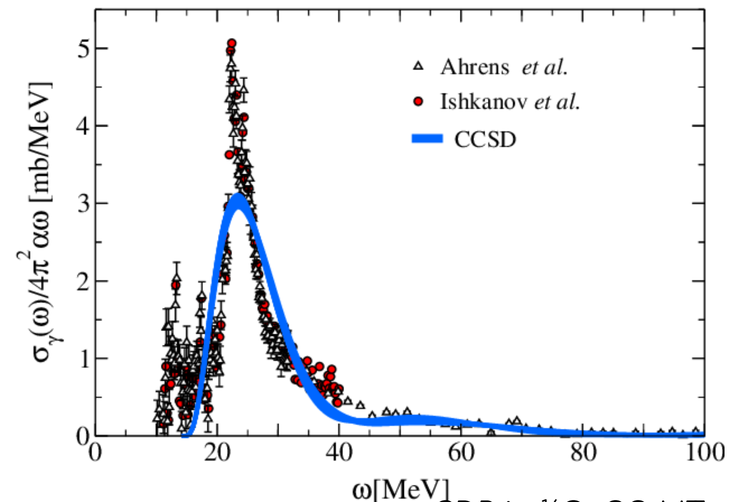

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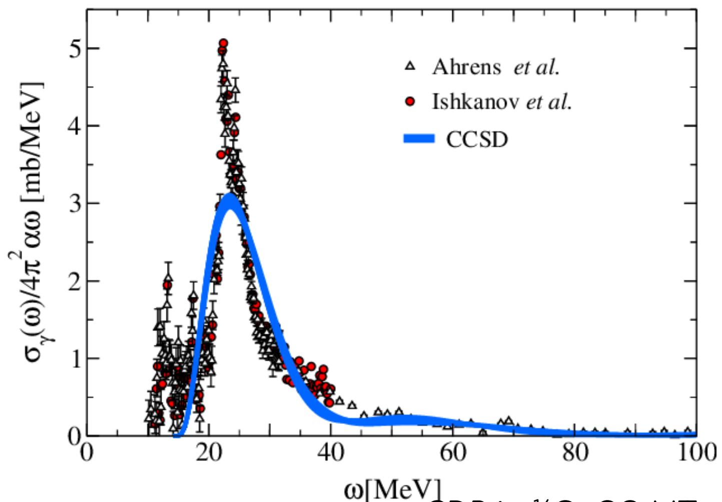

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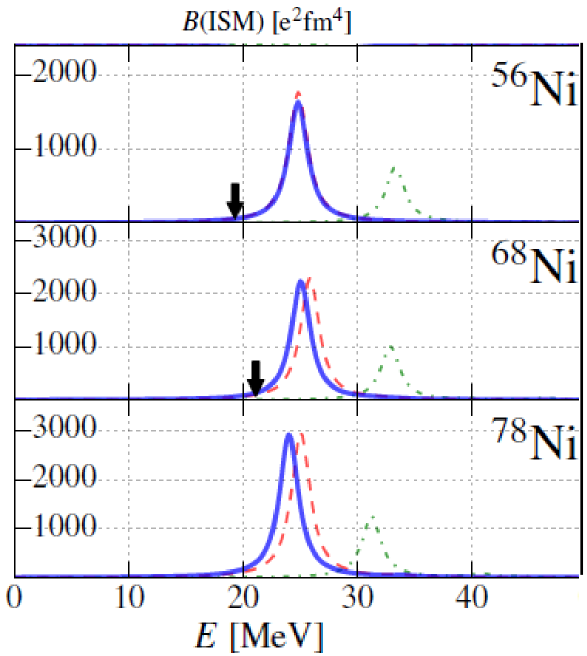

Role of three-body forces

- Systematic effect on the peaks' position
- Crucial aspect in ab-initio
- Different possible treatments

NN-only (-·-·-)
NN+3N-ind. (- - - -)
NN+3N (——)

[From R. Trippel, PhD Thesis, Technischen Universität Darmstadt, 2016]

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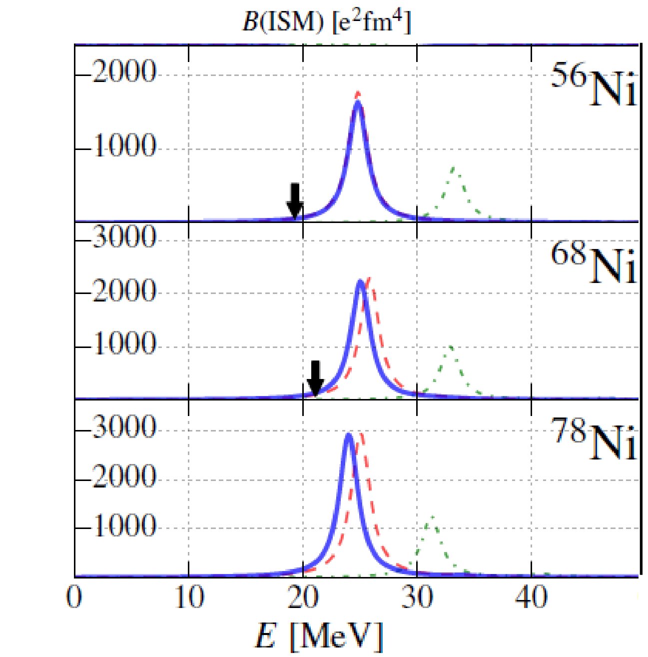

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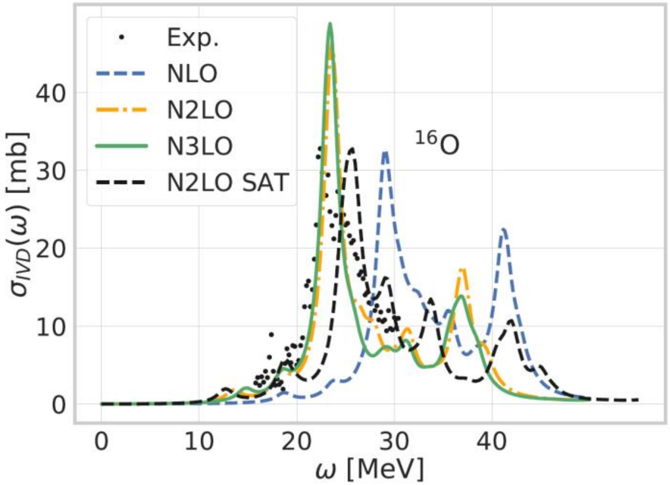

Chiral order dependence

- Convergence wrt the chiral order within given family
- Non-negligible dependence on the used fit
- Good agreement with exp for presently used family

[Y. Beaujeault-Taudière, M. Frosini, J.-P. Ebran, T. Duguet, R. Roth, V. Somà, arXiv:2203.13513]

Ab-initio RPA and beyond

RPA suffers from a congenital disorder

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Quasi-Boson Approximation

Pauli principle violation

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1. First step towards more sophisticated Boson Expansions
2. The HF reference state is NOT the real RPA ground-state

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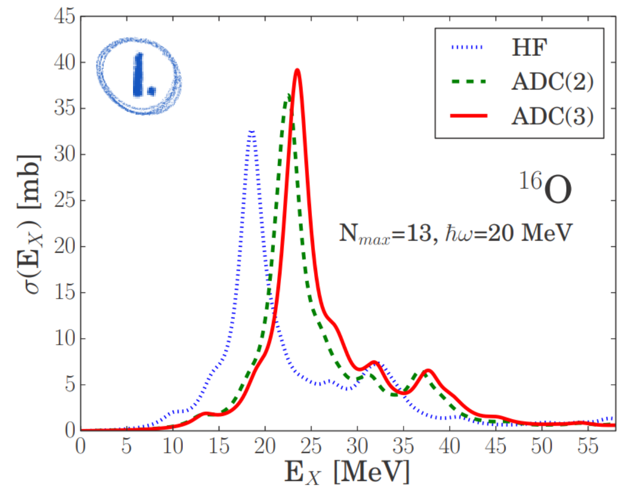

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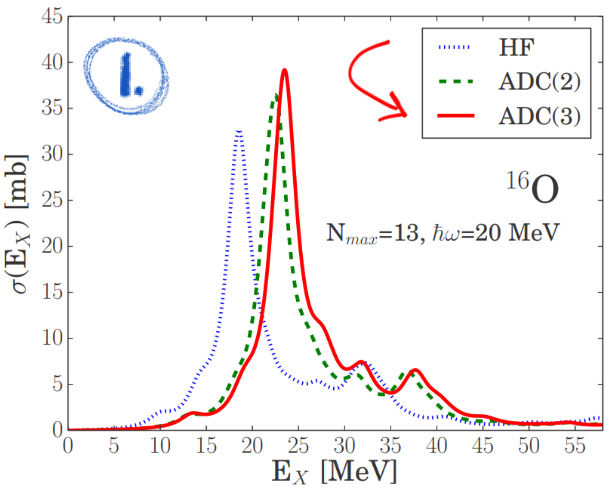

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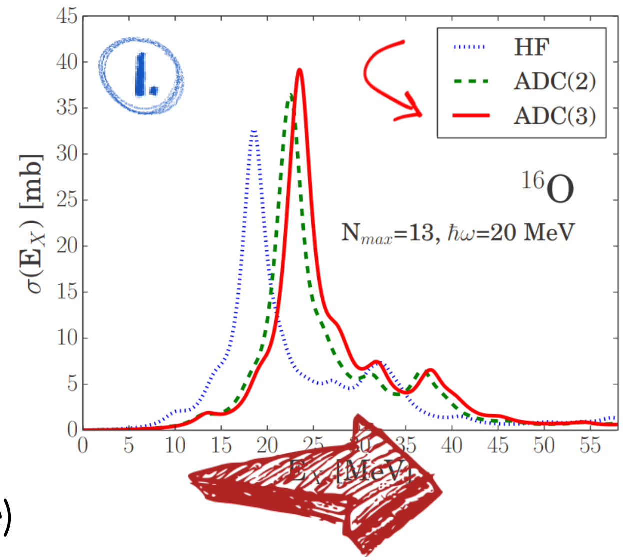
GDR in ^{16}O

[Raimondi, Barbieri, PRC 2019]



GS correlation

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- Going towards the RPA GS via self-consistent RPA (iterative)
- Adding GS correlation lowers the GS (strength shifted up)

Ab-initio RPA and beyond

RPA suffers from a congenital disorder

Quasi-Boson Approximation

Pauli principle violation

(But this is often asymptomatic)

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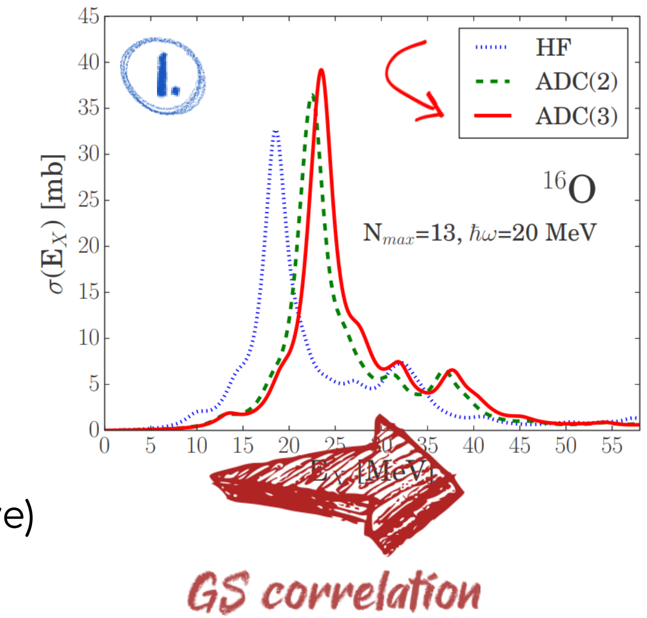

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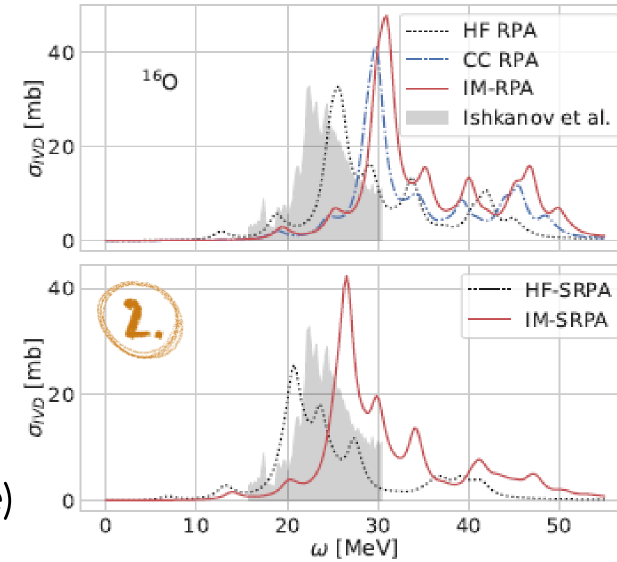

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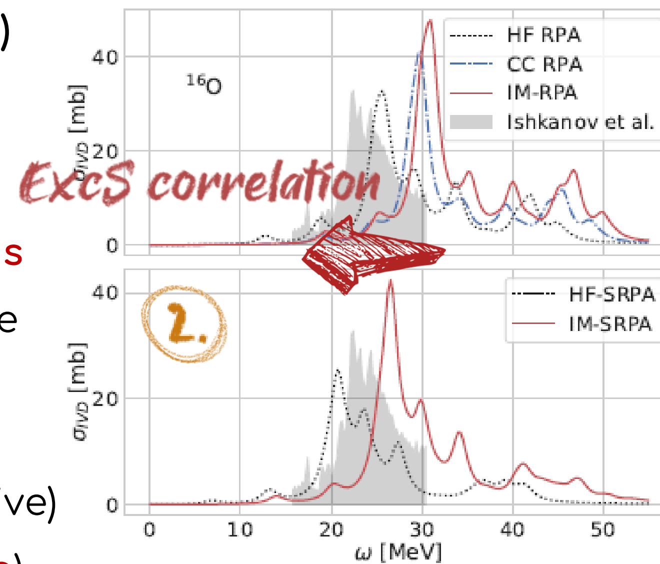

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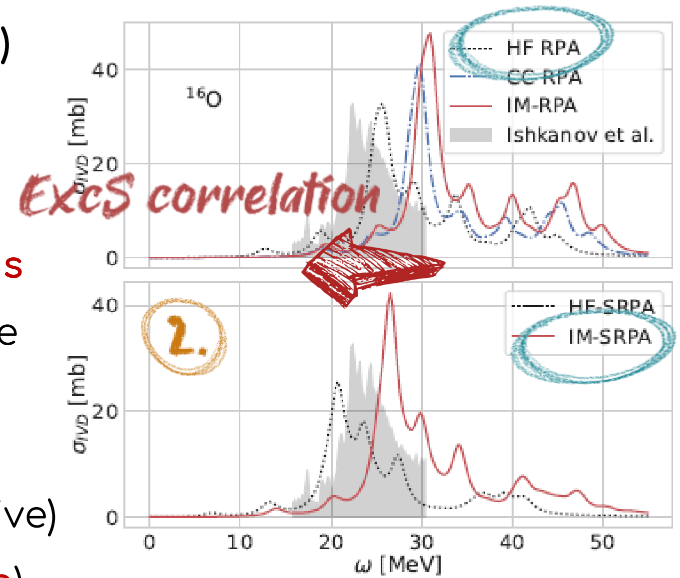

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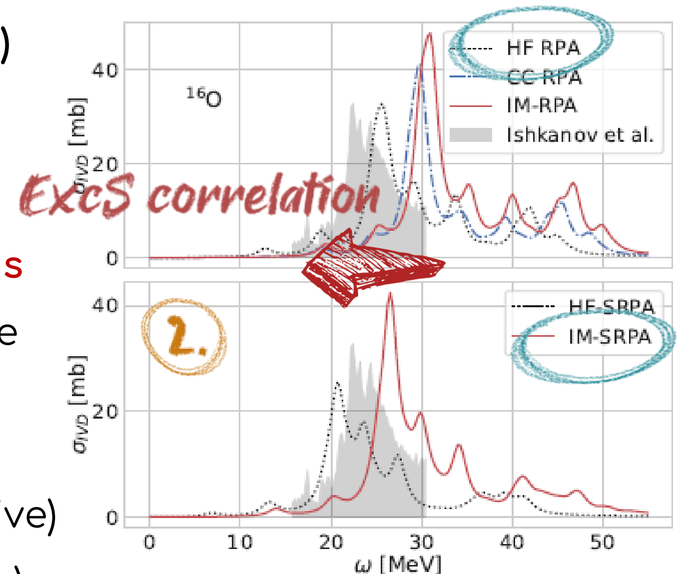

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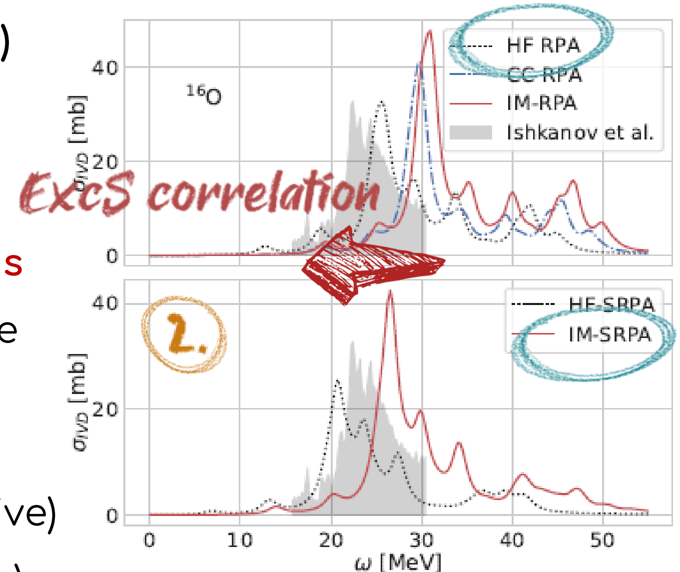

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Valid motivation for ab-initio RPA !

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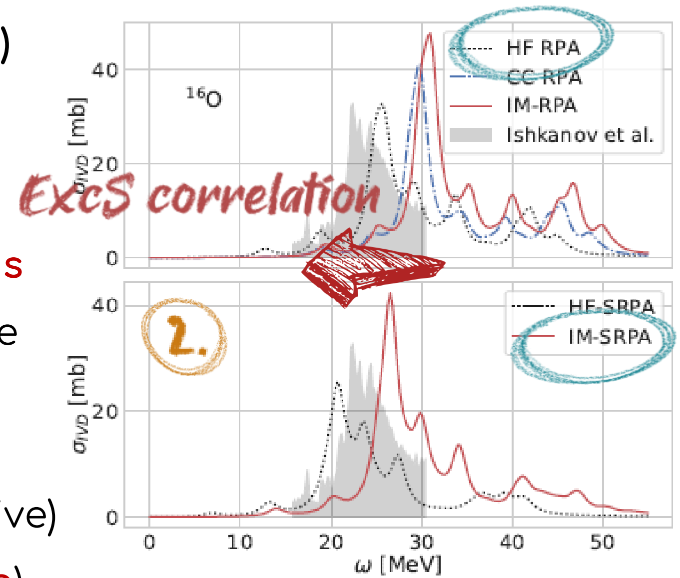

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Well known issue in Quantum Chemistry

G_0W vs GW approximation

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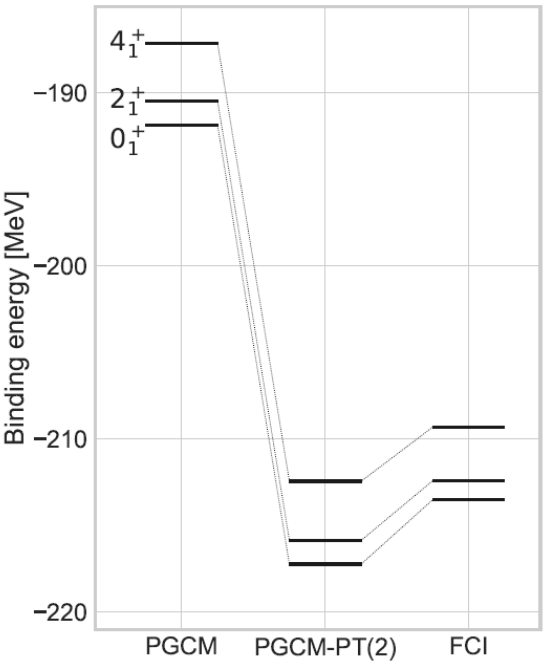
Correlation in PGCM



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- Perturbation theory + PGCM (PGCM-PT) recently formulated
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[Frosini et al. , EPJA, 2022]

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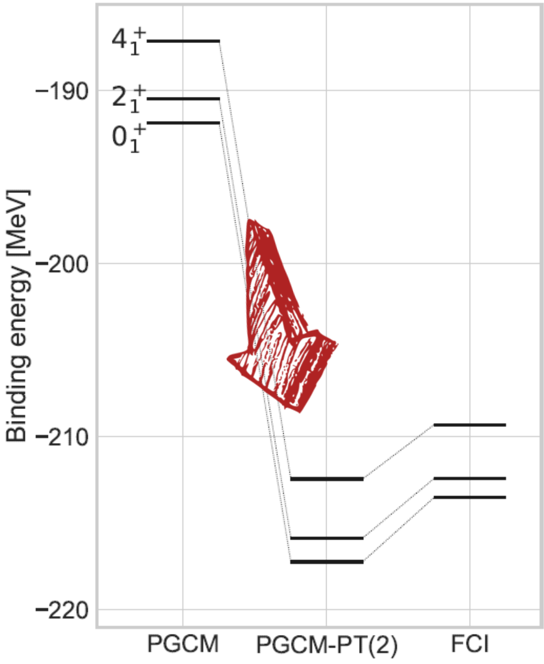

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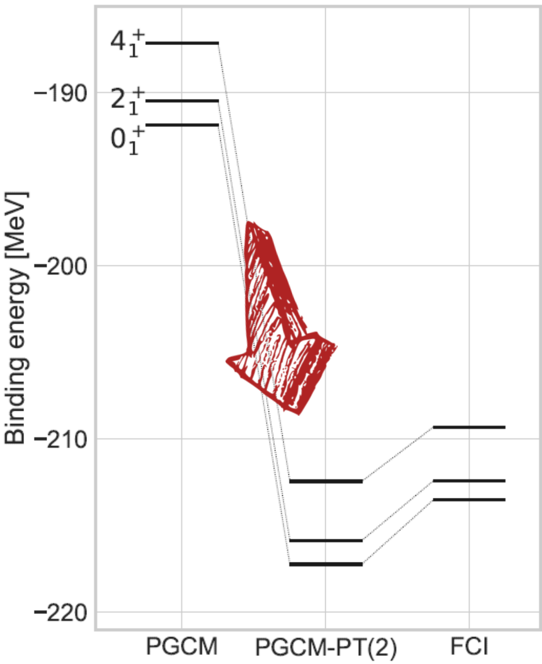

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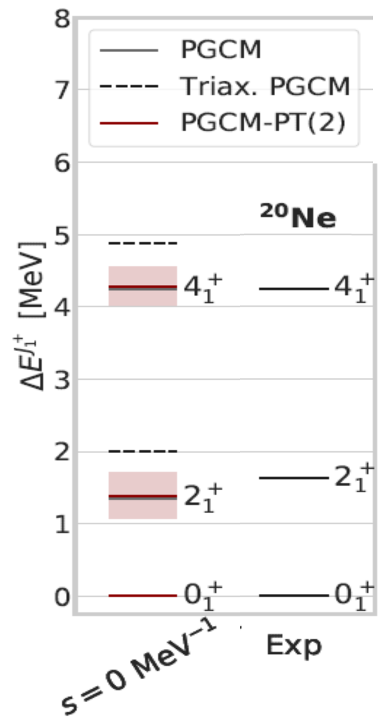

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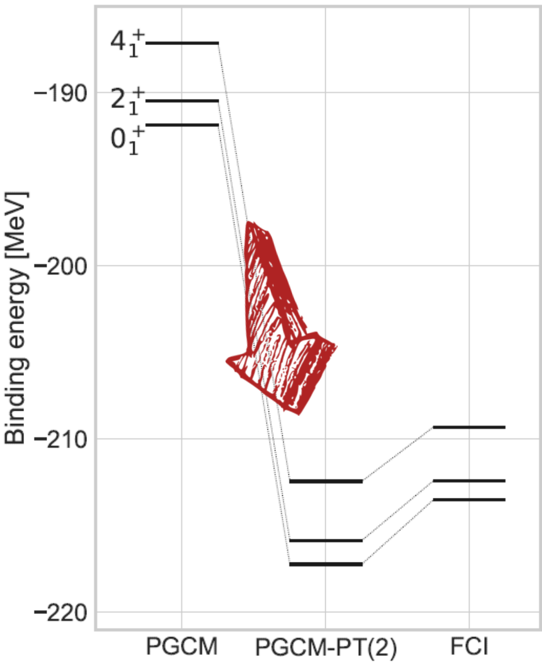

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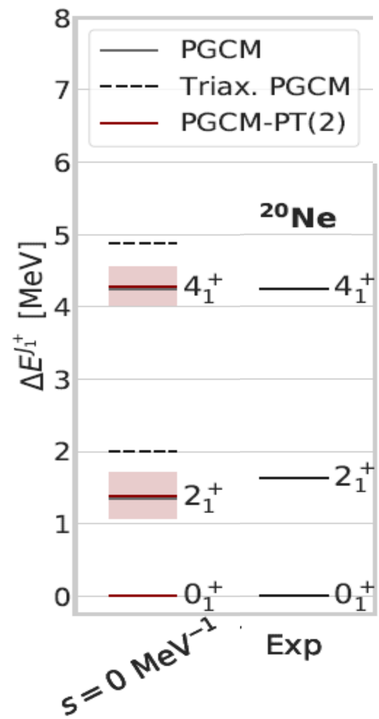

Error cancellation for spectroscopy !

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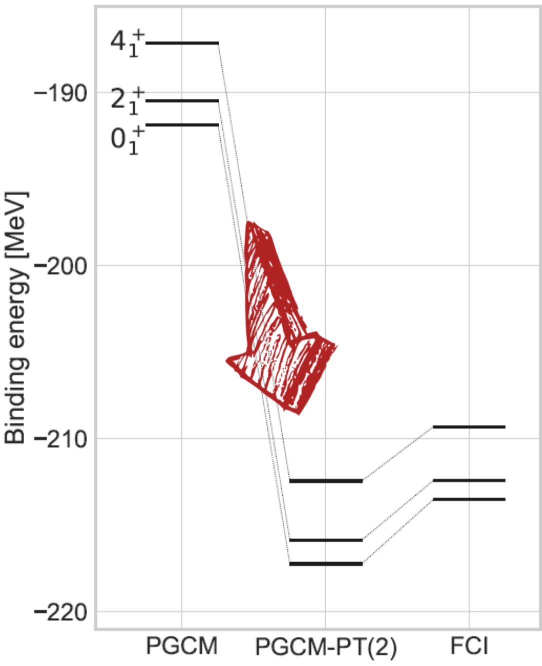

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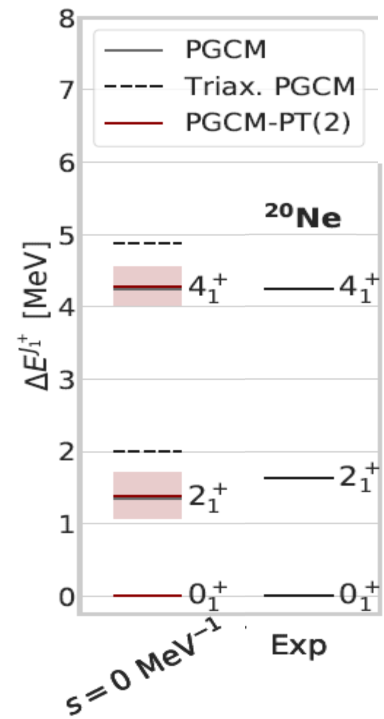

Error cancellation for spectroscopy !

PGCM promising ab-initio candidate for collective ecxs

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What to (and not to) expect ?
(From the present talk/study)

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- Closed- and open-shell nuclei
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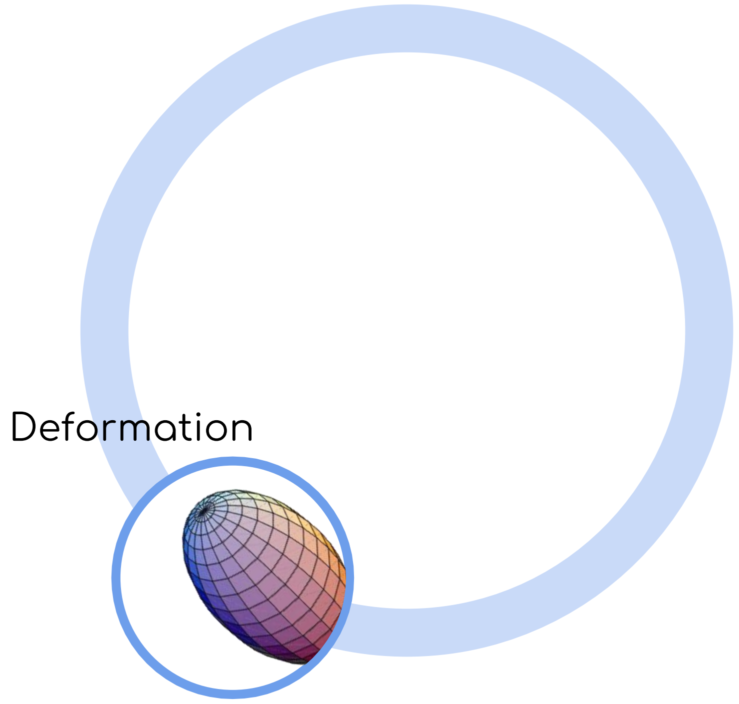

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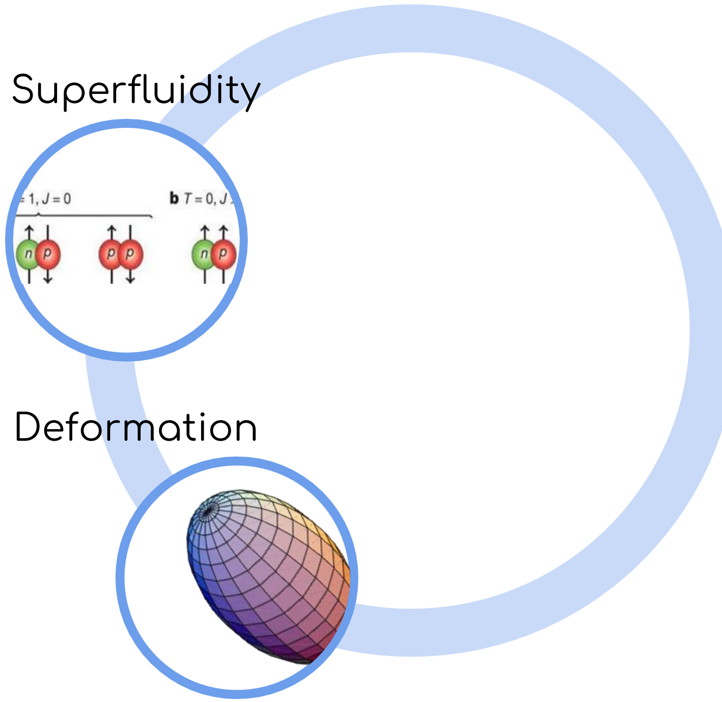

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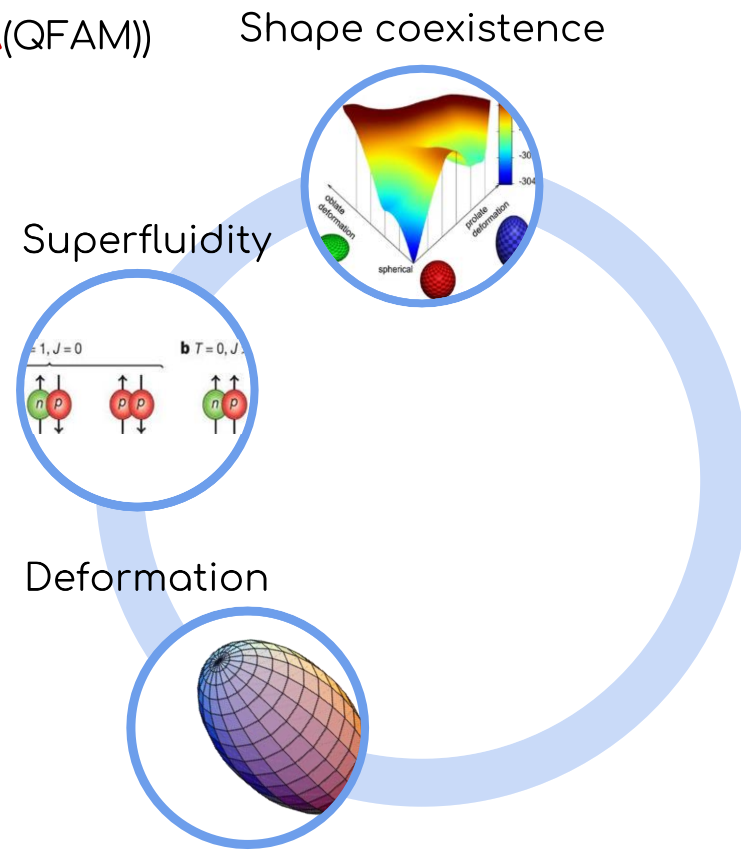

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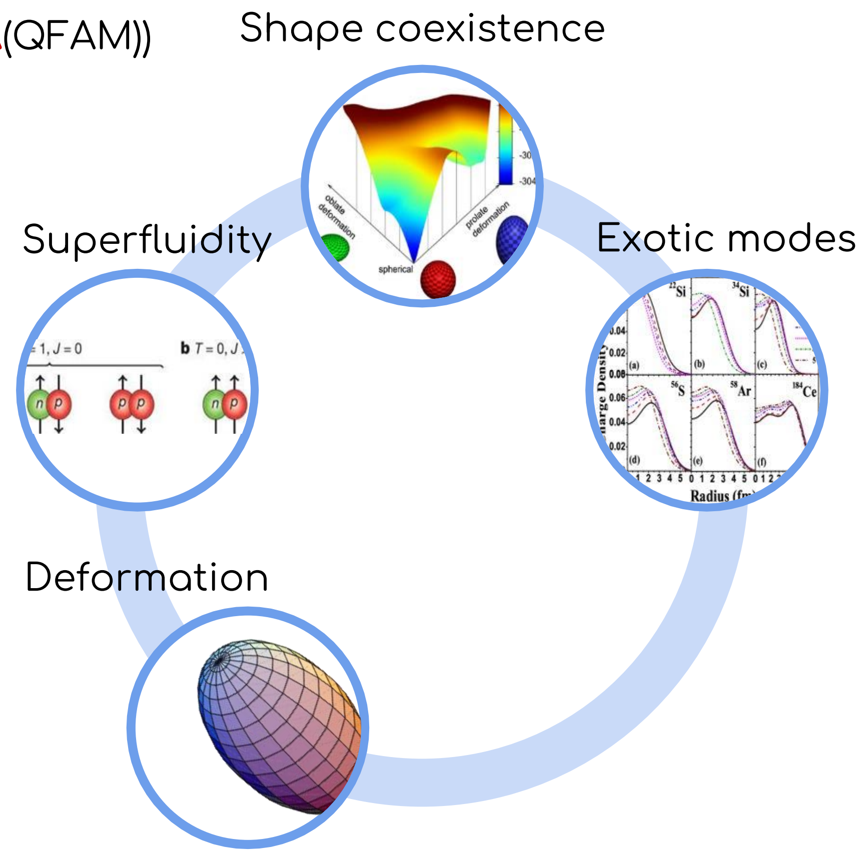

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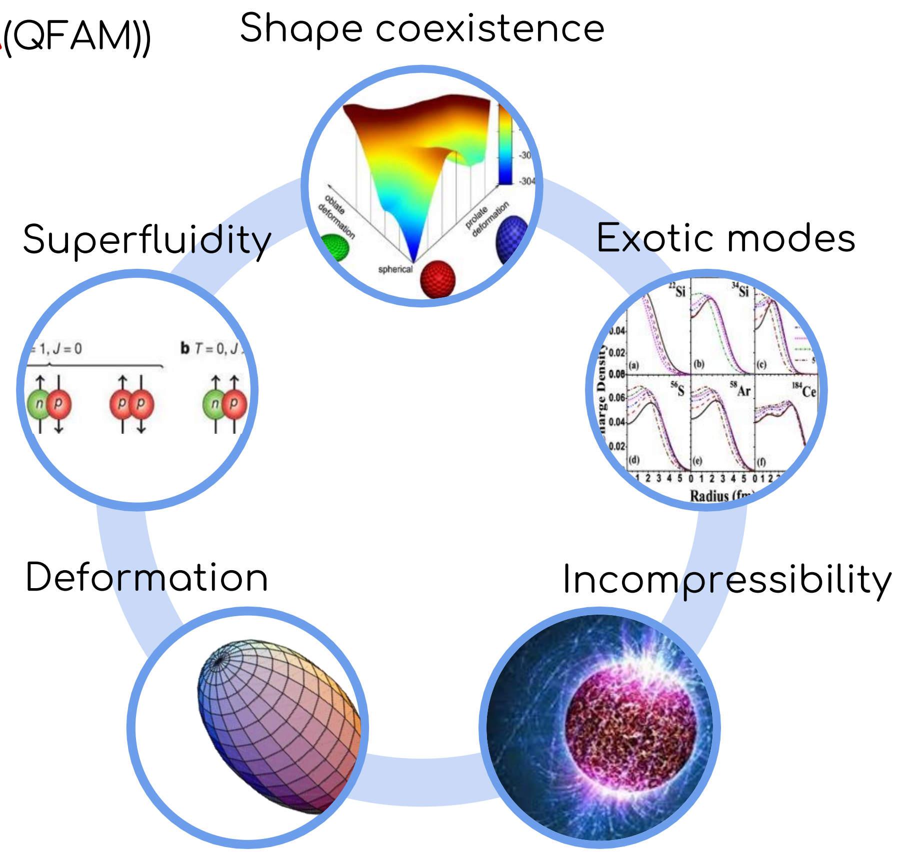

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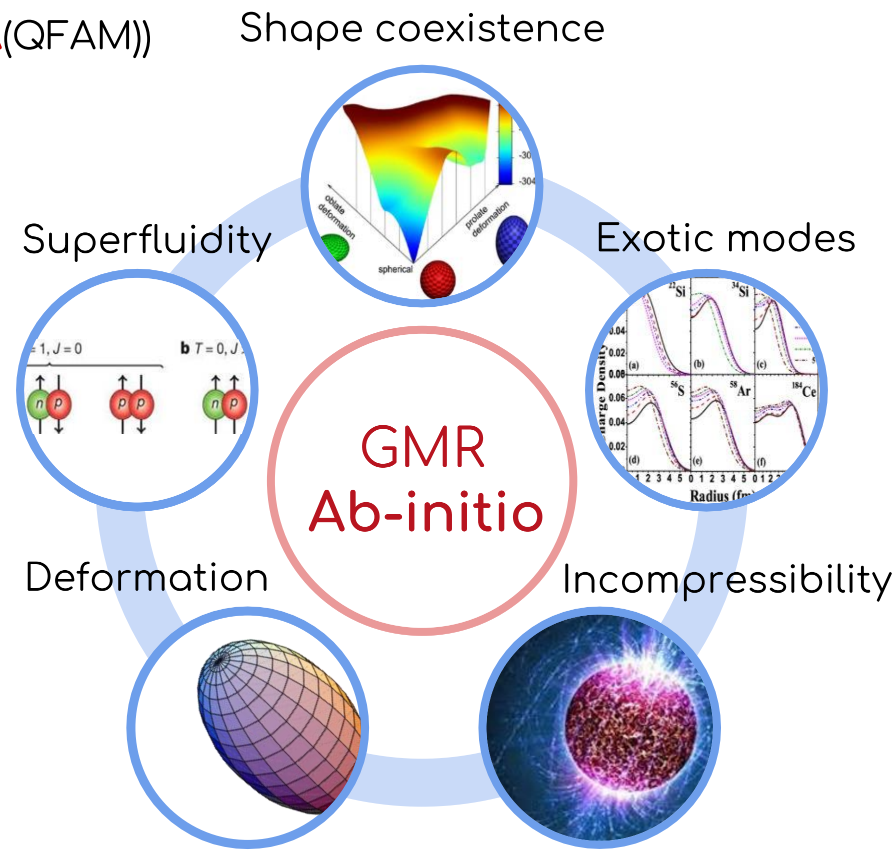

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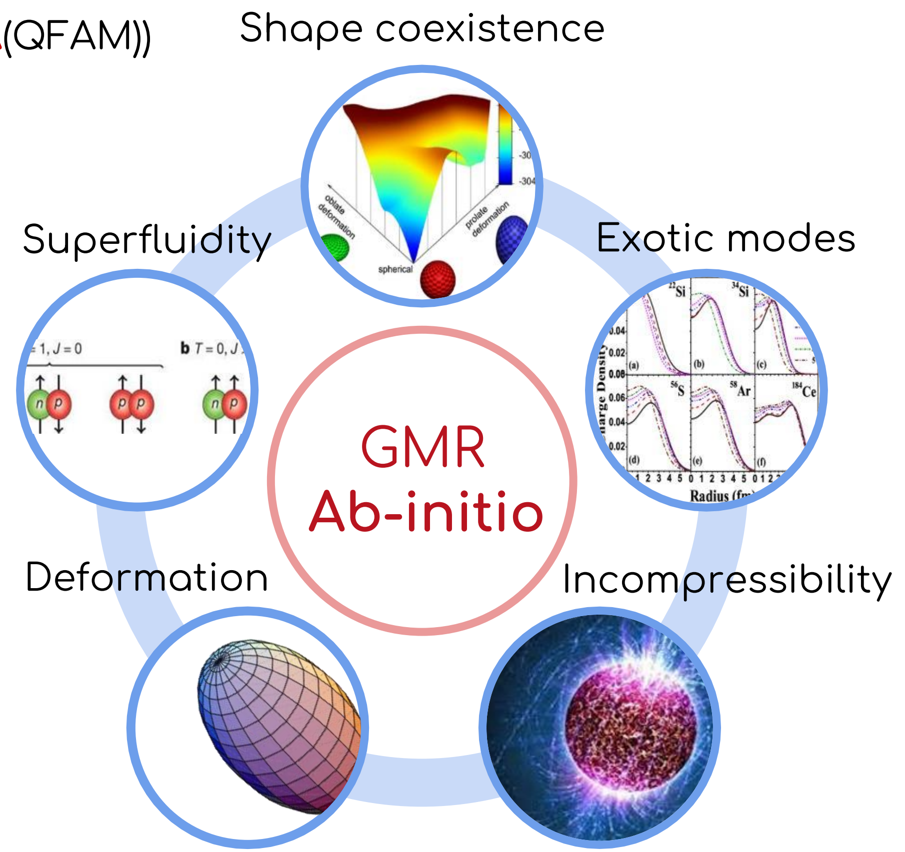

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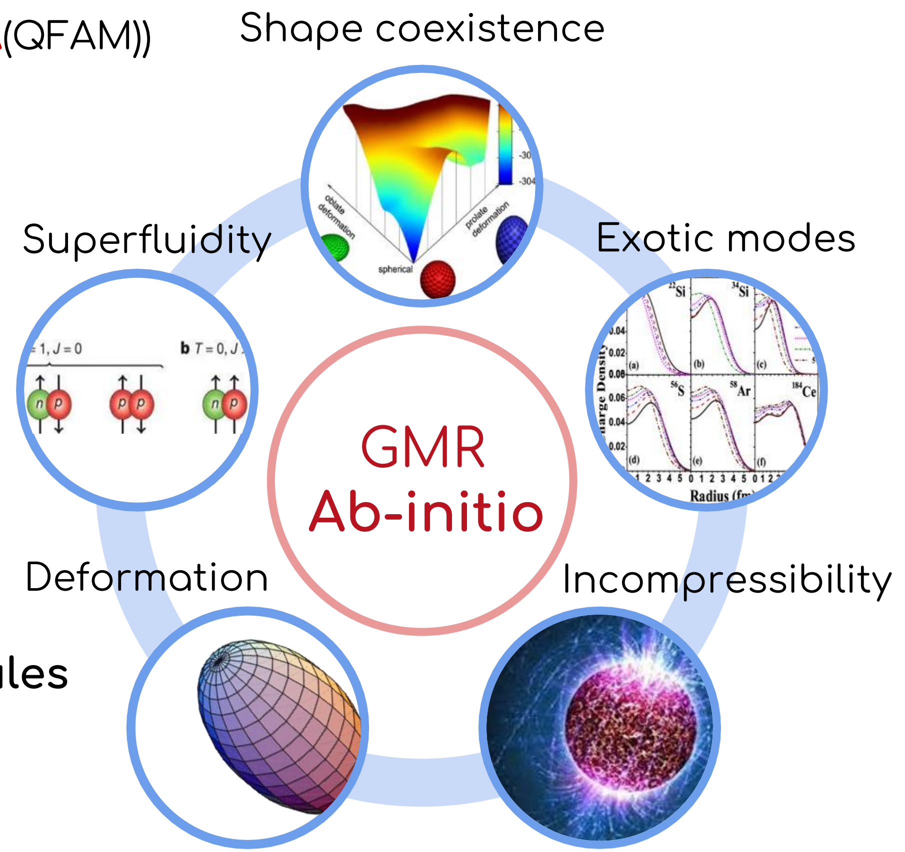

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- Pairing/isospin effects «fluffiness»

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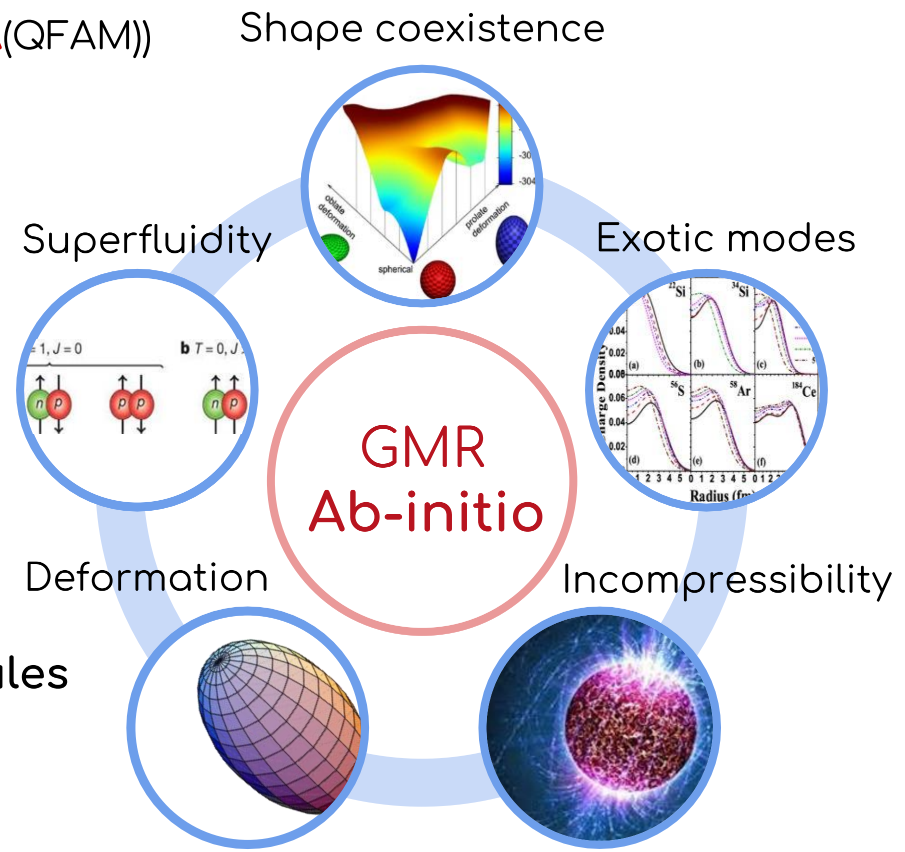

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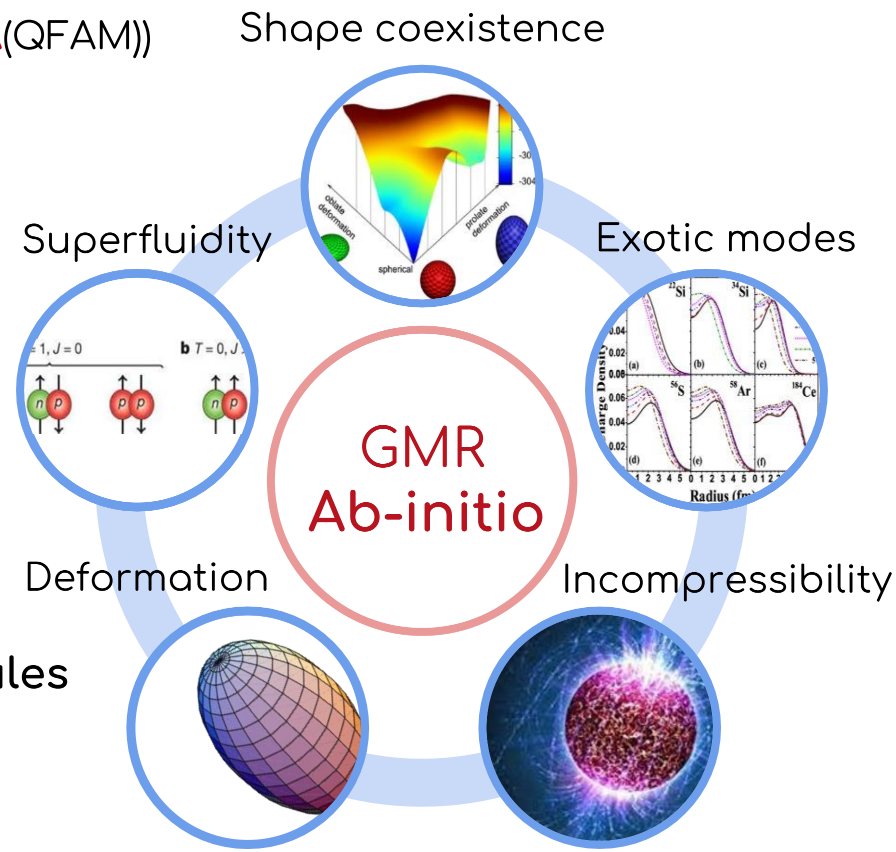

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Ni isotopes and more systematics coming soon !

Outline

- Introduction
- **Formalism**
  - Ab-initio PGCM and QFAM for GMR
- Preliminary results
- Conclusions

PGCM

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

PGCM

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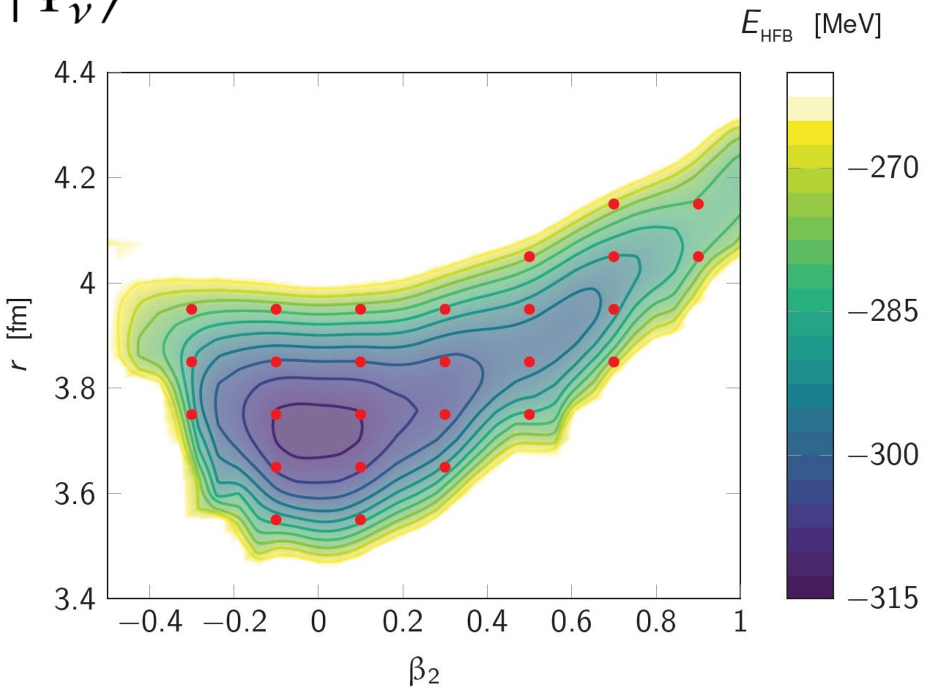
1 Constrained HFB solutions

$|\Phi(r^2, \beta_2)\rangle$



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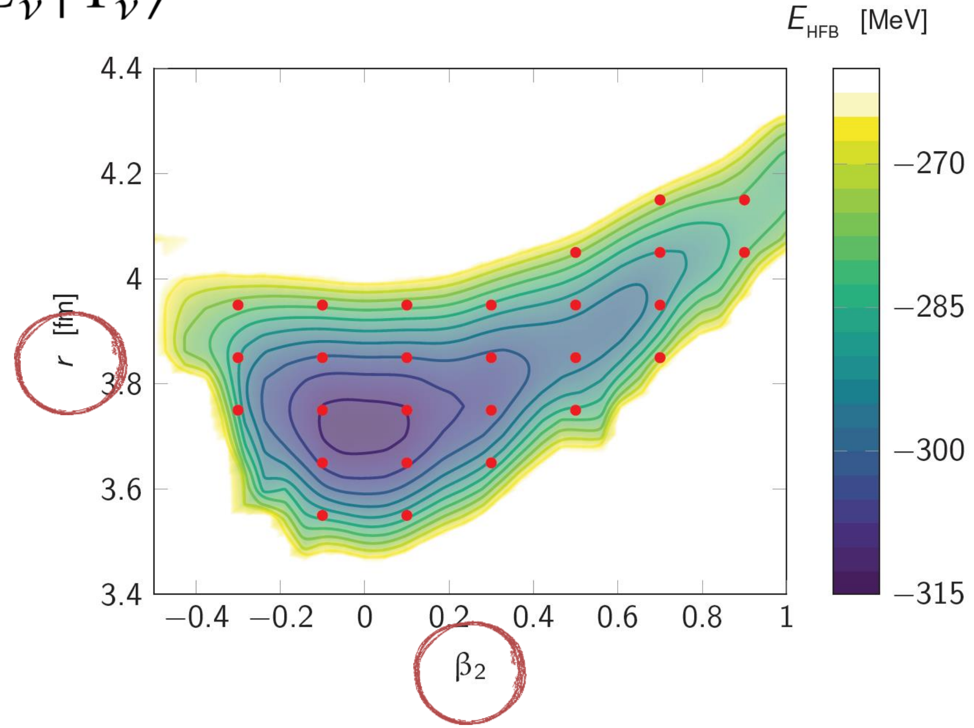
Generator coordinates «q»



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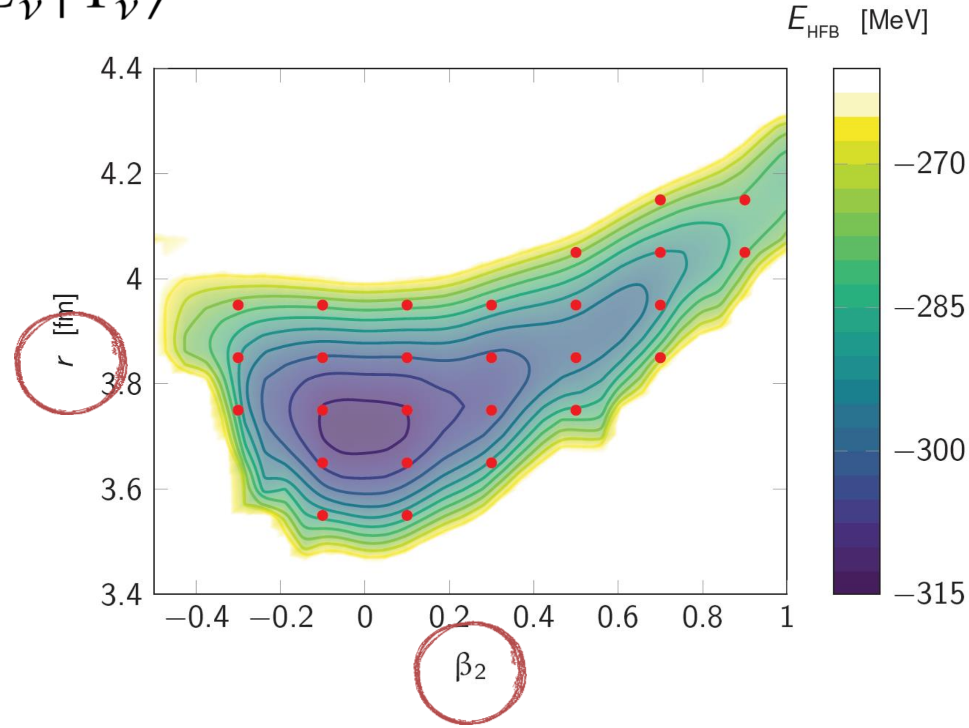

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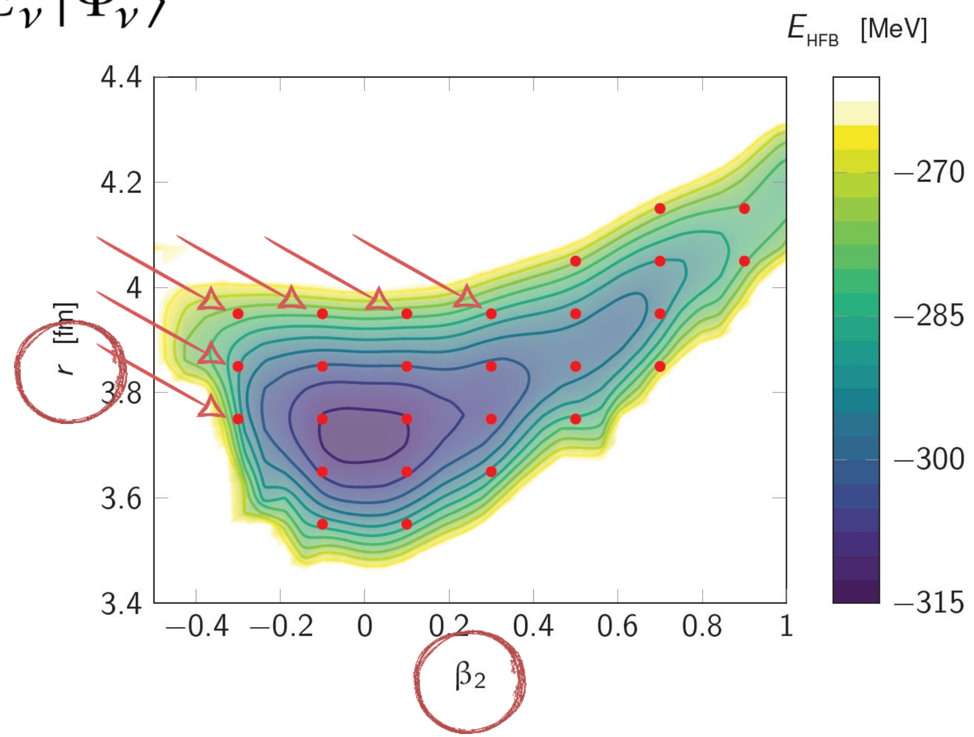

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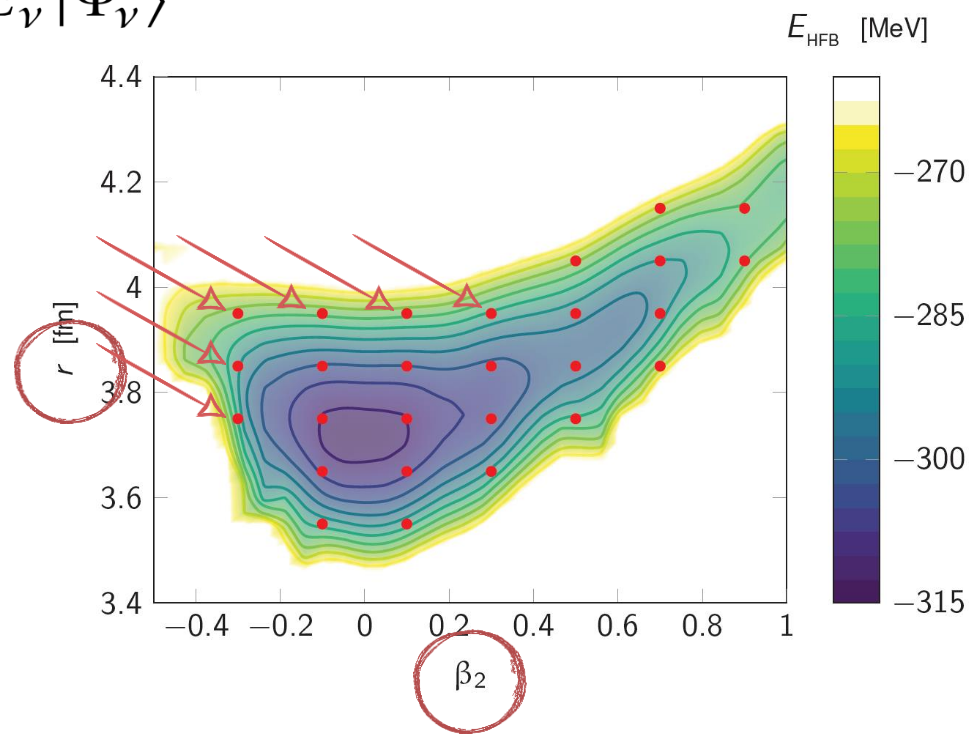

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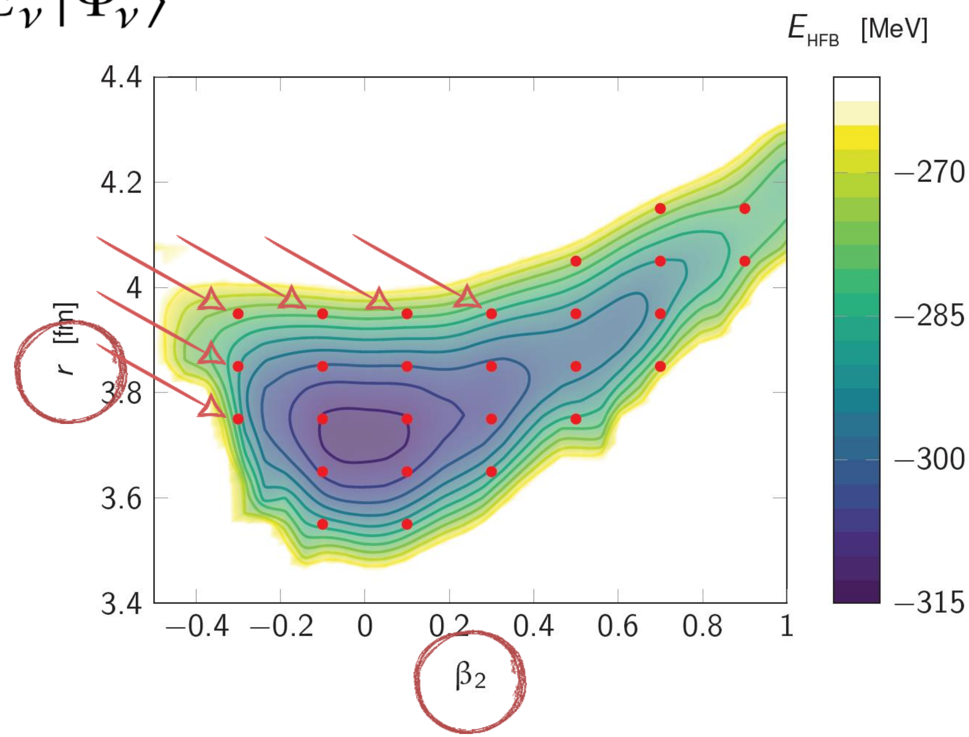
$$\delta \frac{\langle\Psi_\nu|H|\Psi_\nu\rangle}{\langle\Psi_\nu|\Psi_\nu\rangle} = 0$$

Variational method



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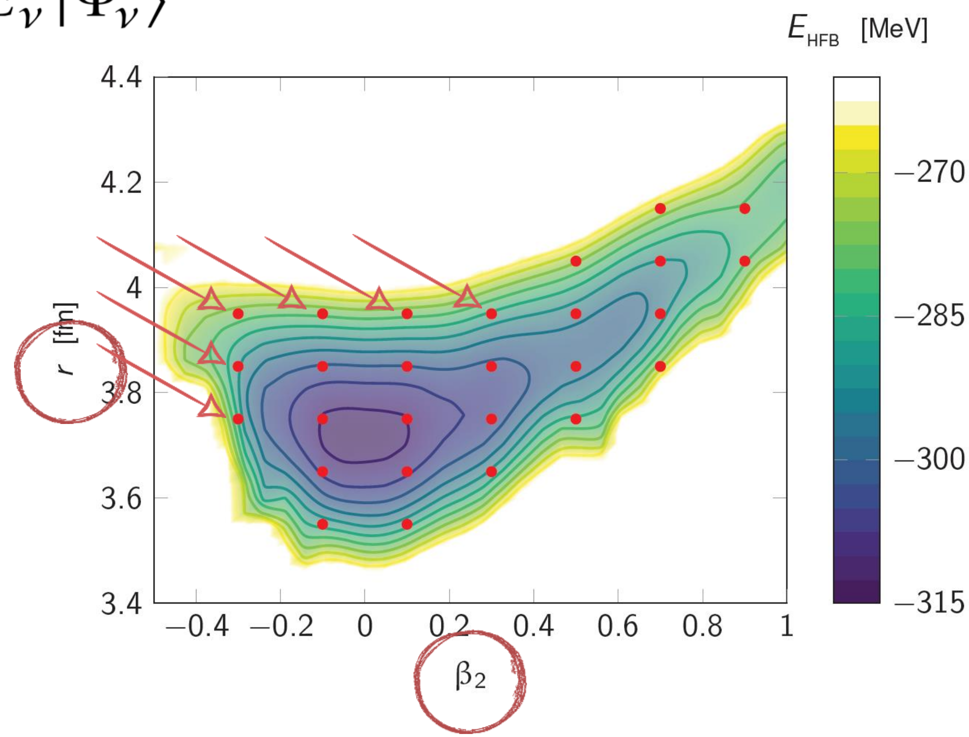
Variational method

$$\sum_q \left[\mathcal{H}(p,q) - E_\nu\mathcal{N}(p,q)\right] f_\nu(q) = 0$$

Schrödinger-like equation



Kernels evaluation

$$\mathcal{H}(p,q) \equiv \langle\Phi(p)|H|\Phi(q)\rangle$$
$$\mathcal{N}(p,q) \equiv \langle\Phi(p)|\Phi(q)\rangle$$

[Ring, Schuck, The nuclear many-body problem (1980)]

[Porro, Duguet, arXiv:2206.03781]

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Generator coordinates «q»

2 PGCM Ansatz

$$|\Psi_\nu\rangle = \sum_{r^2,\beta_2} f_\nu(r^2,\beta_2)|\Phi(r^2,\beta_2)\rangle$$

Linear coefficients

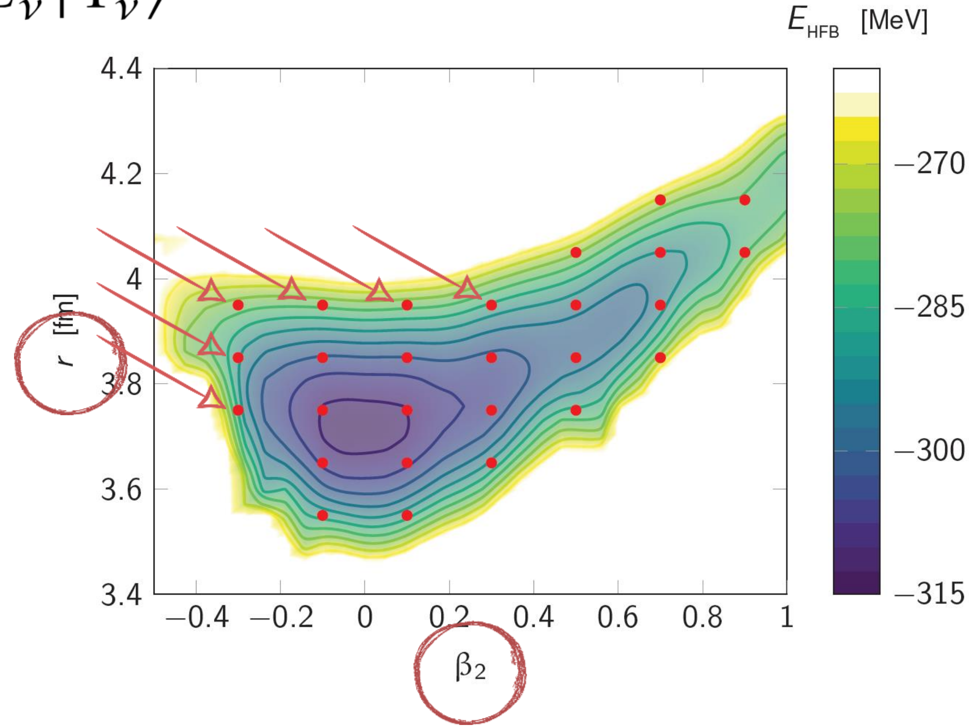
3 HWG Equation

$$\delta\frac{\langle\Psi_\nu|H|\Psi_\nu\rangle}{\langle\Psi_\nu|\Psi_\nu\rangle} = 0$$

Variational method

$$\sum_q\left[\mathcal{H}(p,q) - E_\nu\mathcal{N}(p,q)\right]f_\nu(q) = 0$$

Schrödinger-like equation



Kernels evaluation

$$\mathcal{H}(p,q) \equiv \langle\Phi(p)|H|\Phi(q)\rangle$$
$$\mathcal{N}(p,q) \equiv \langle\Phi(p)|\Phi(q)\rangle$$

[Ring, Schuck, The nuclear many-body problem (1980)]

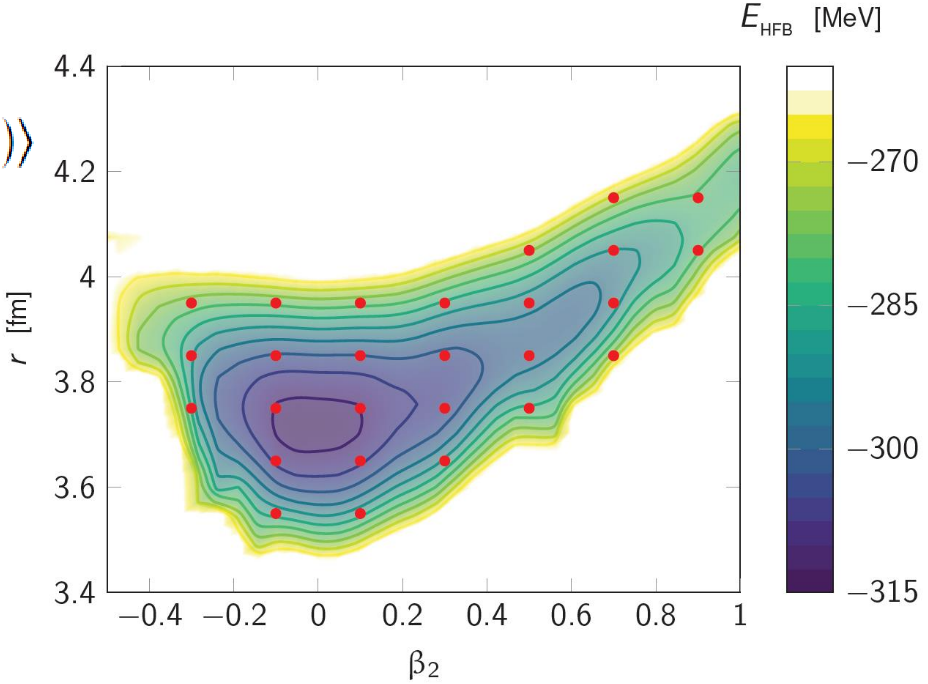
[Porro, Duguet, arXiv:2206.03781]

Diagonalization in a reduced Hilbert space

(Q)RPA from GCM

Thouless theorem

$$|\Phi(q)\rangle = \langle\Phi(q_{min})|\Phi(q)\rangle \, e^{\mathbf{Z}(q,q_{min})} \, |\Phi(q_{min})\rangle$$



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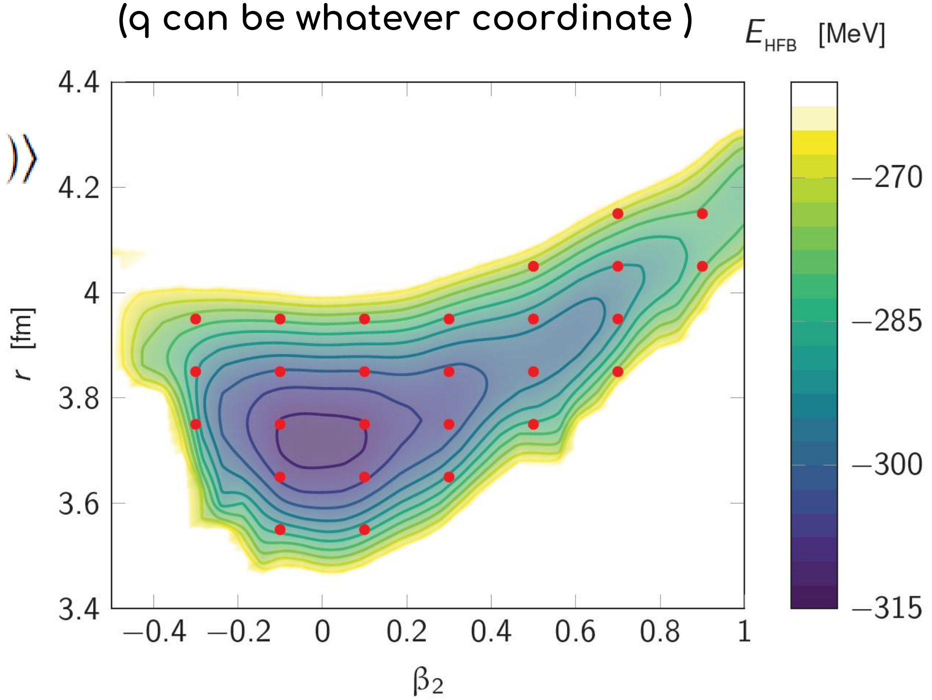
(q can be whatever coordinate)



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Non-unitary transformation

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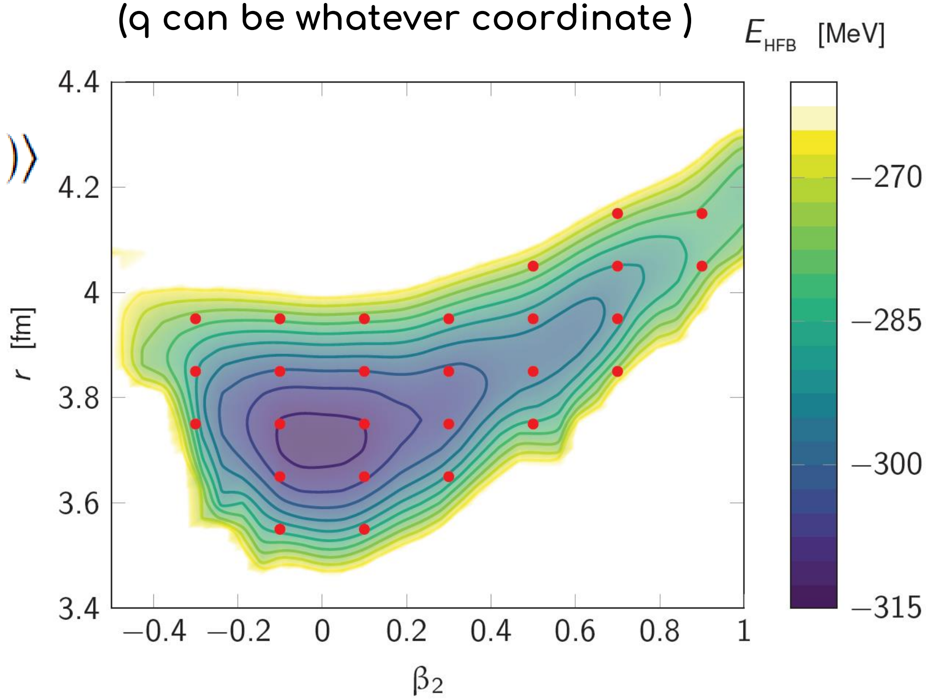

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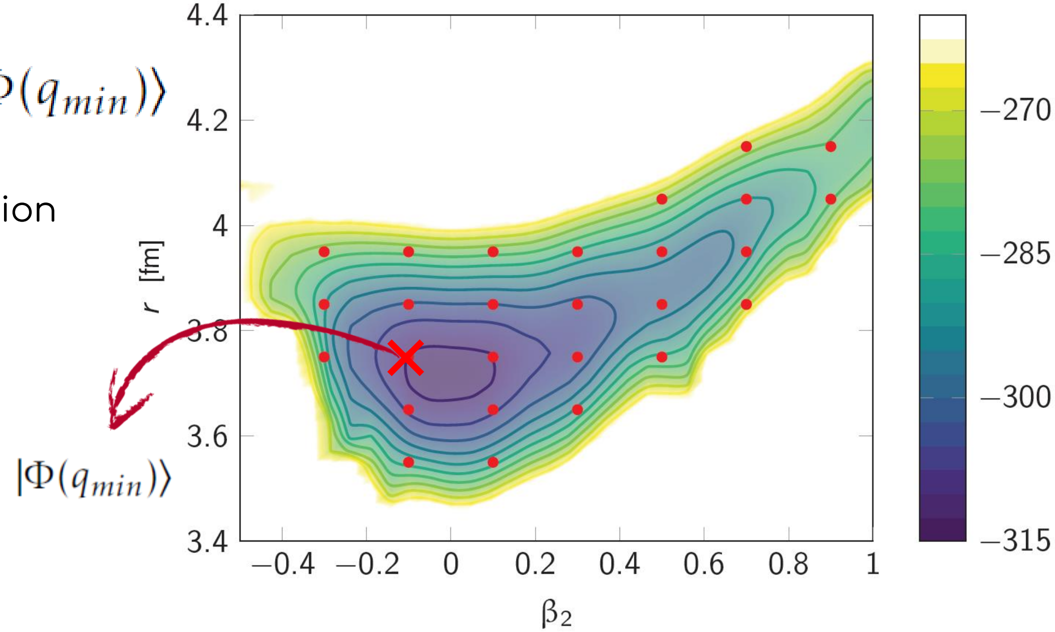

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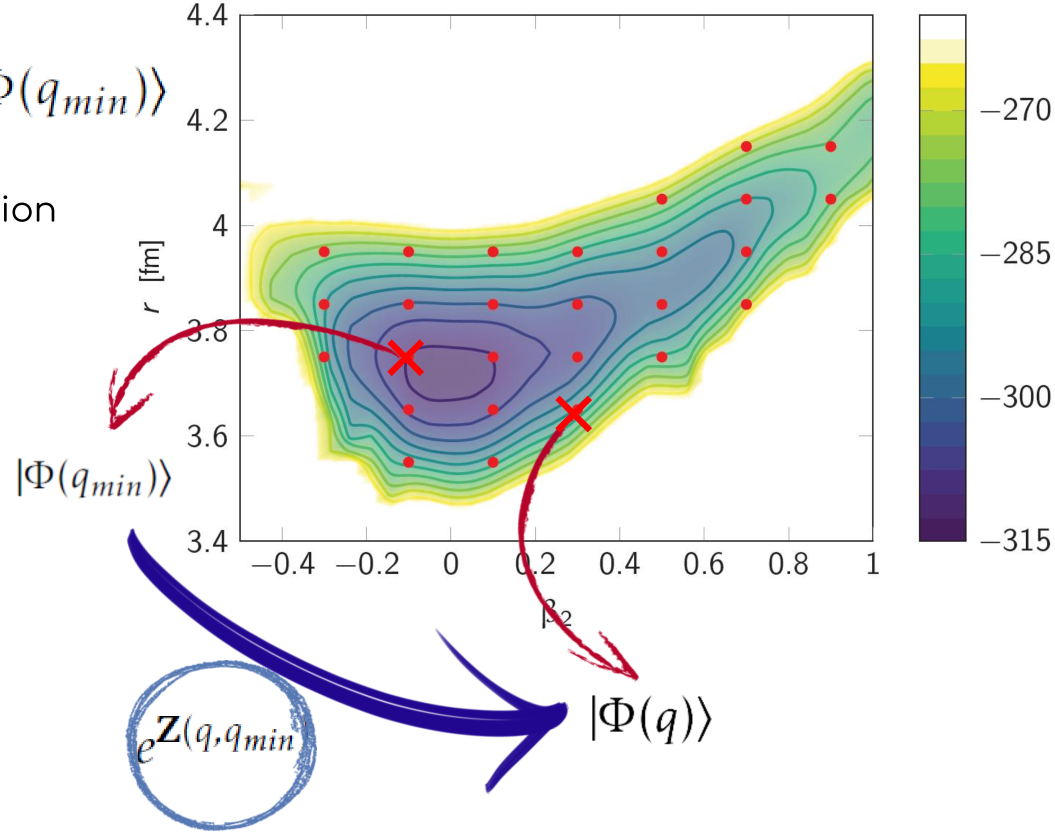

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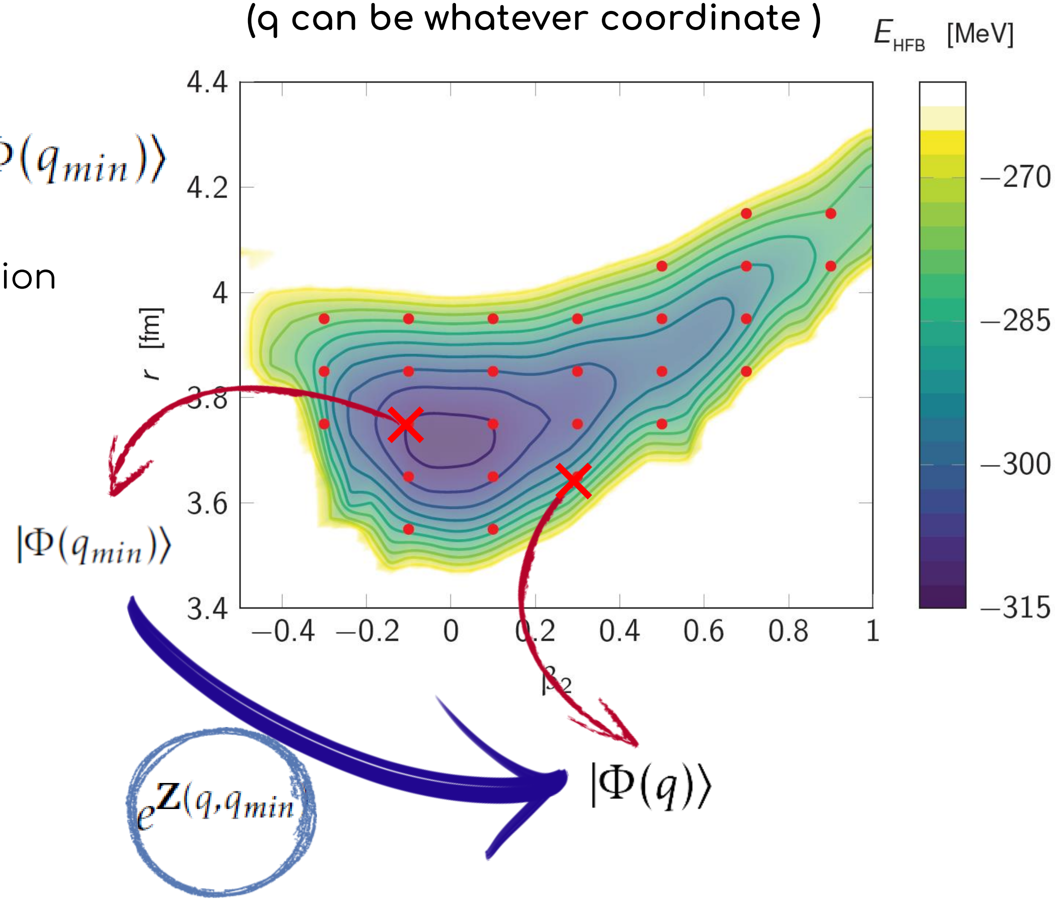

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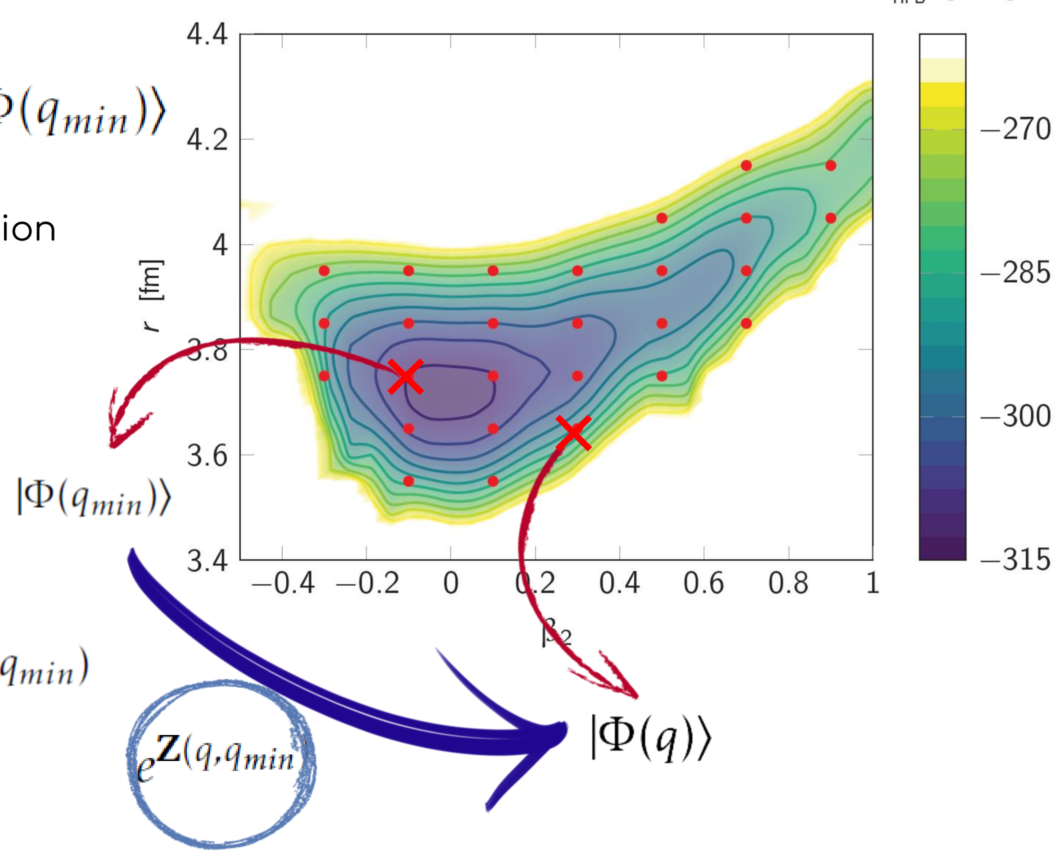

HWG Equation

$$\delta \frac{\langle\Psi_\nu|H|\Psi_\nu\rangle}{\langle\Psi_\nu|\Psi_\nu\rangle} = 0$$

Solve with **two approximations**:

- QBA
- Expand to the quadratic level in $\mathbf{Z}(q,q_{min})$

  → Harmonic approximation

(Q)RPA from GCM

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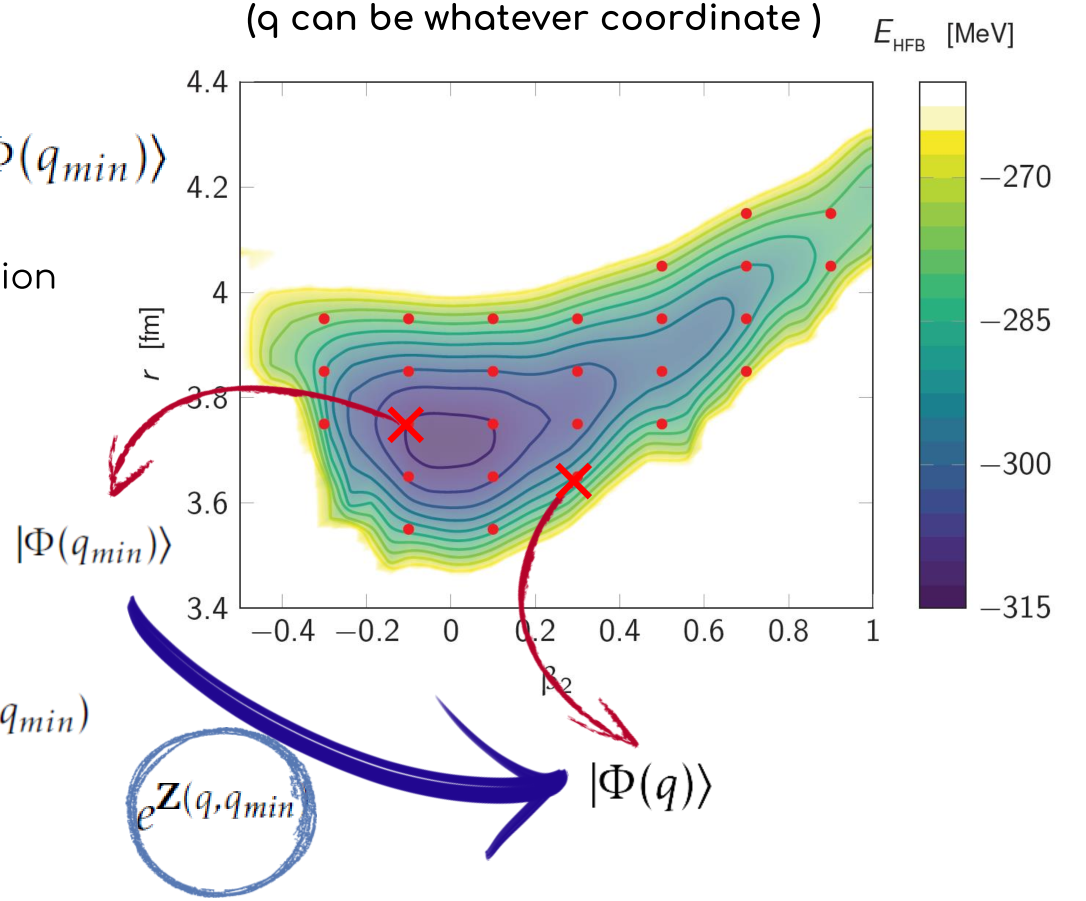

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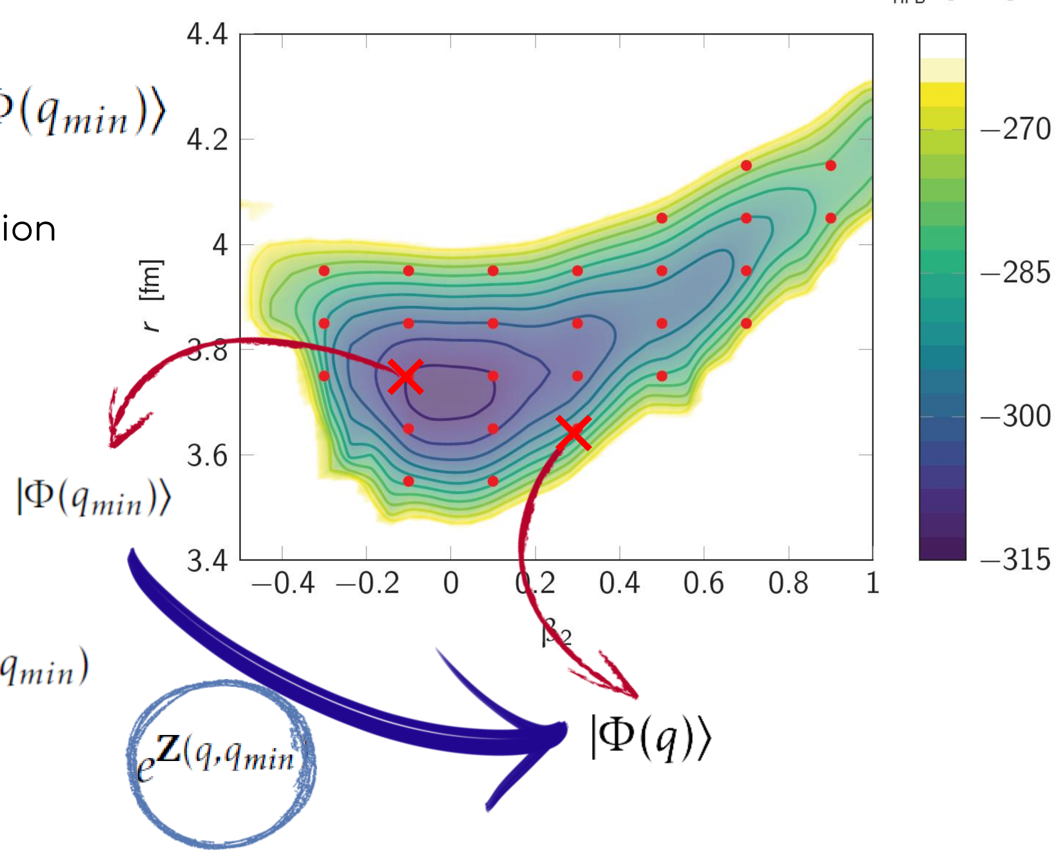

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No coordinates dependency !

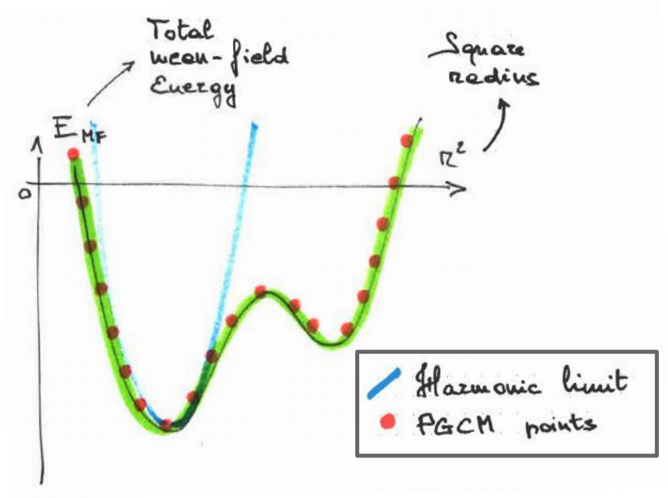
Eventually rewrites as QRPA

[Jancovici, Schiff, 1964]

$$\begin{pmatrix} A & B \\ -B^* & -A^* \end{pmatrix}\begin{pmatrix} X^\nu \\ Y^\nu \end{pmatrix} = E_\nu \begin{pmatrix} X^\nu \\ Y^\nu \end{pmatrix}$$

PGCM vs QRPA

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



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Schrödinger equation $$H\,|\Psi_\nu\rangle = E_\nu\,|\Psi_\nu\rangle$$

PGCM

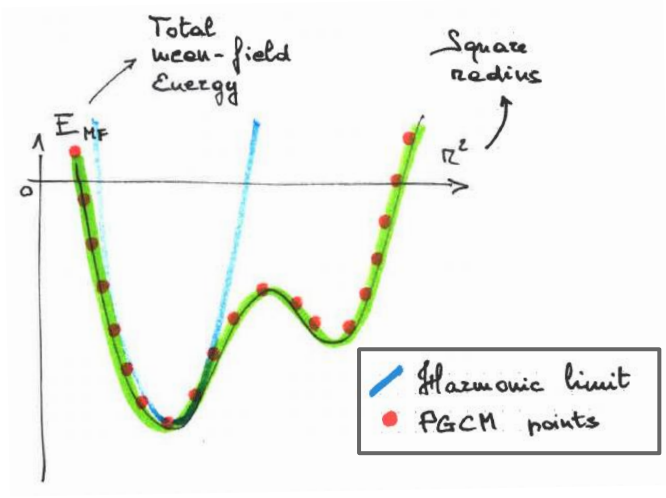
$$|\Psi_\nu\rangle \equiv \sum_{r^2,q} f_\nu(r^2,q)\,|\Phi(r^2,q)\rangle$$

r^2 to study GMR

q to couple to other modes

Symmetry breaking and restoration

Variational method



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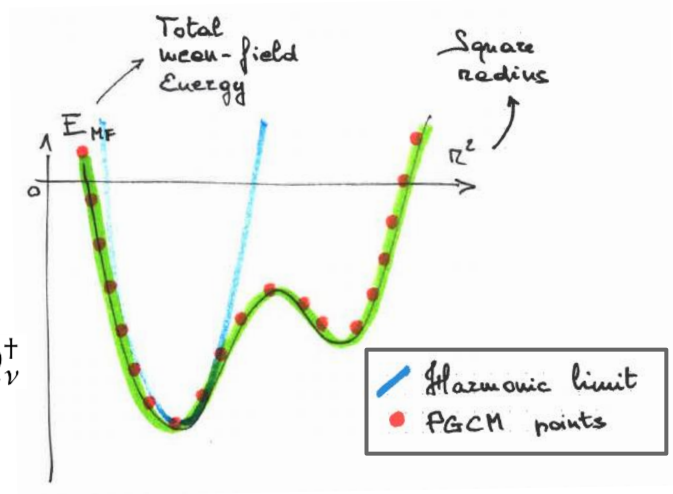
Boson-like excitation operators $Q_\nu^\dagger$

QRPA matrix diagonalization

QFAM formulation frequencies $\mathbb{C}$



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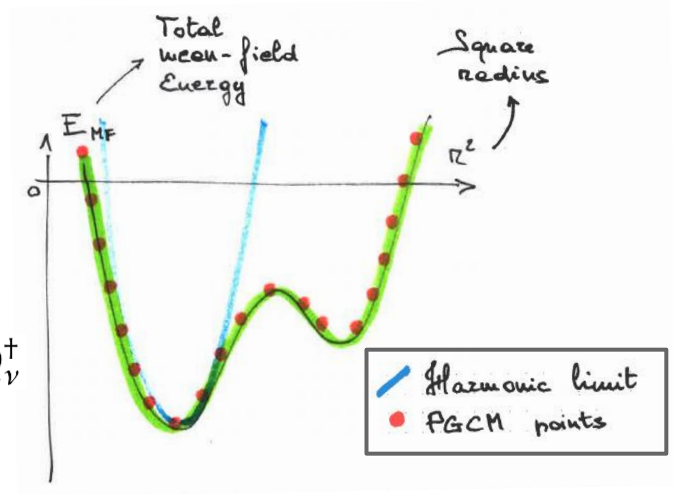

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Pros and Cons

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
Computationally expensive	Low computational cost

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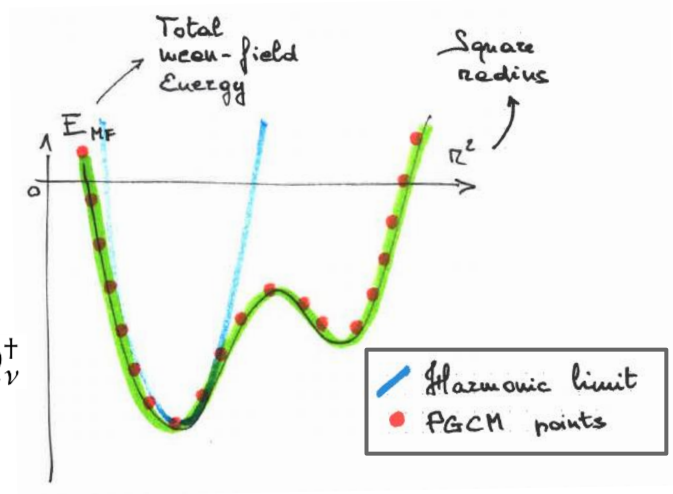

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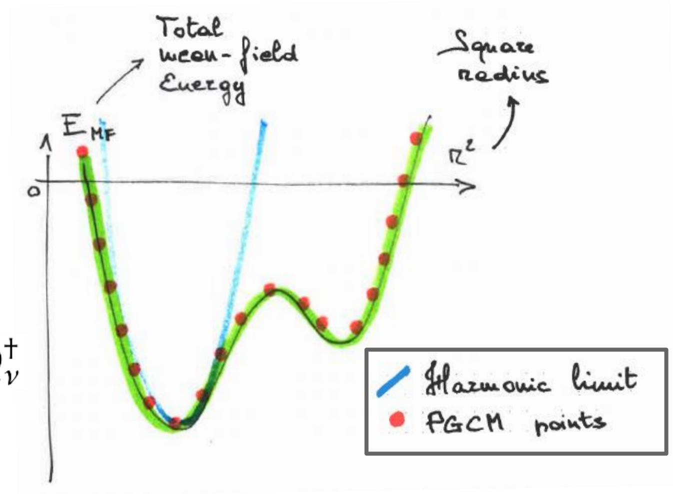

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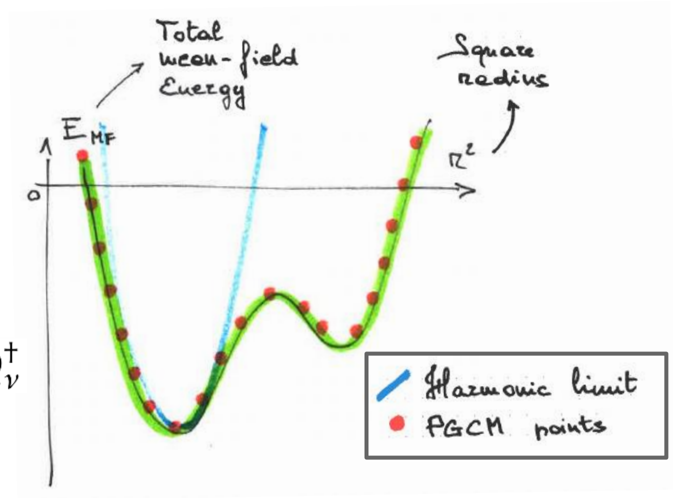

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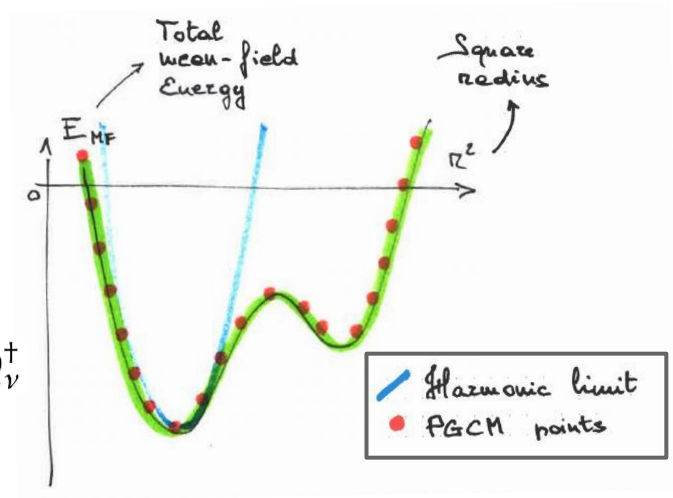

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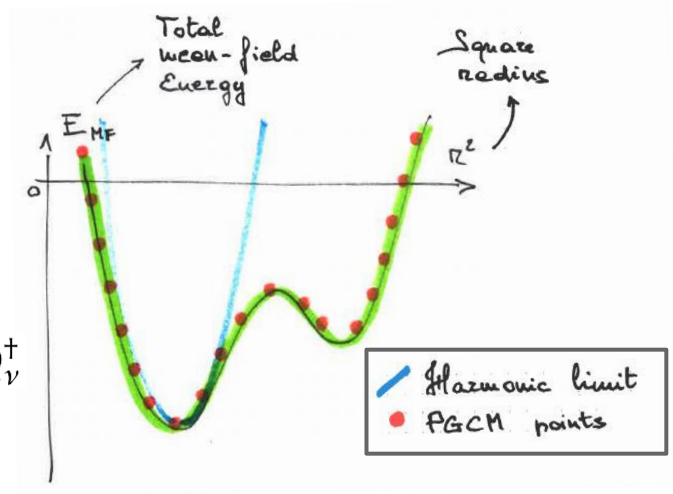

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First ab-initio realization very recently developed

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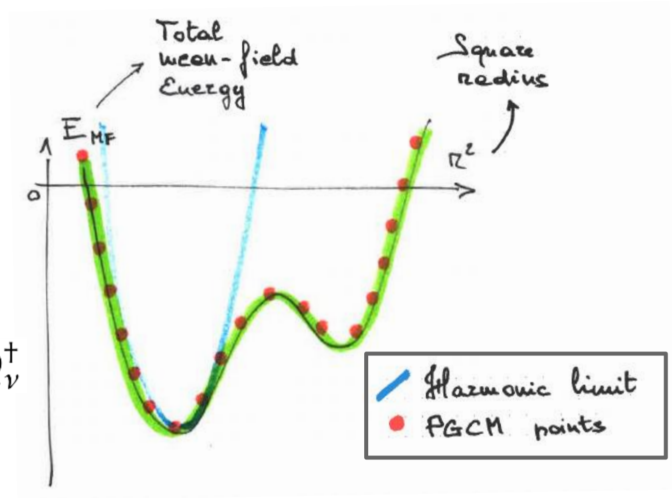

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General implementation, can access

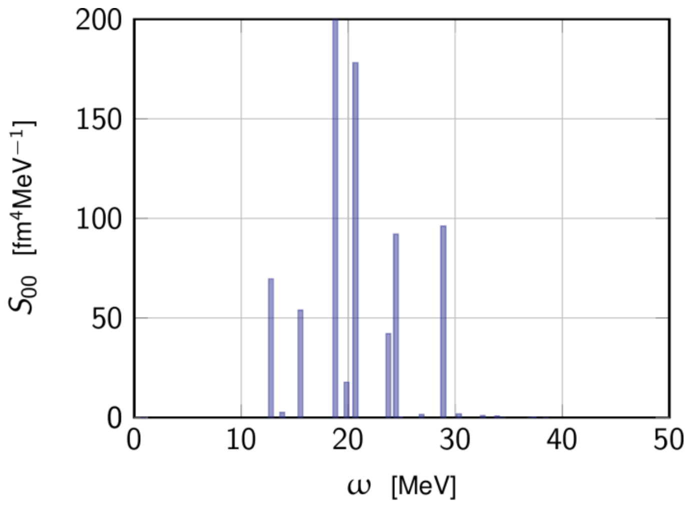
1. Doubly-closed-shell nuclei
2. Singly-open-shell nuclei
3. Doubly-open-shell nuclei

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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JM=00

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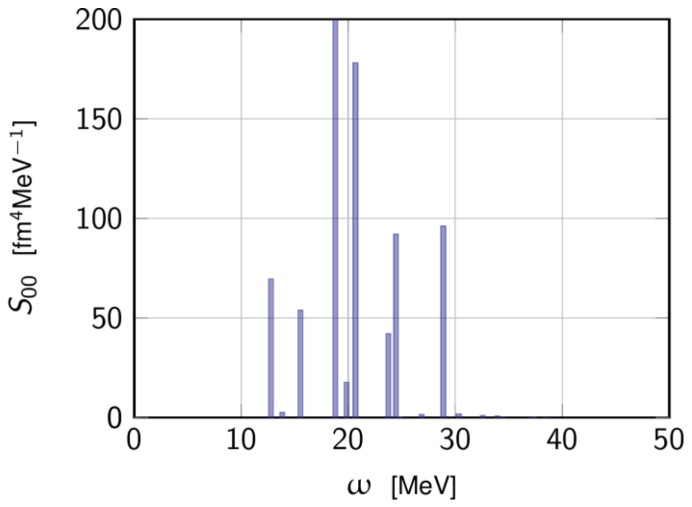

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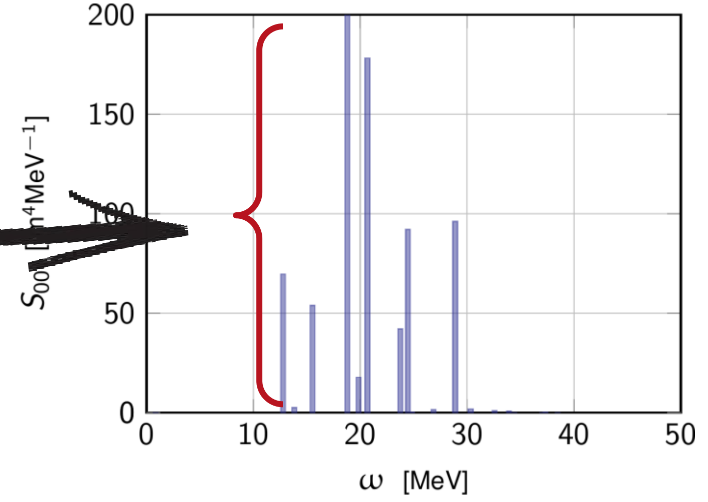

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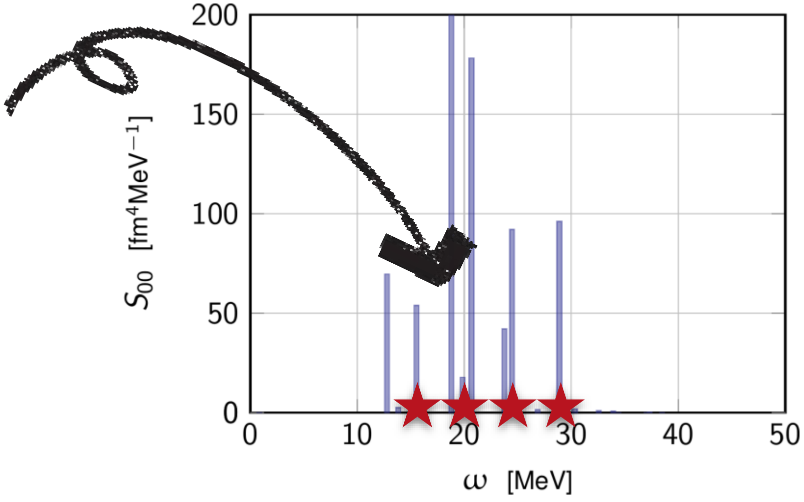

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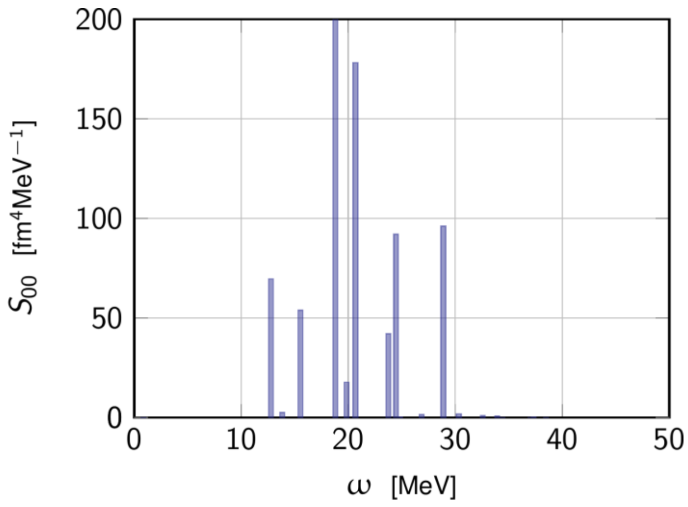

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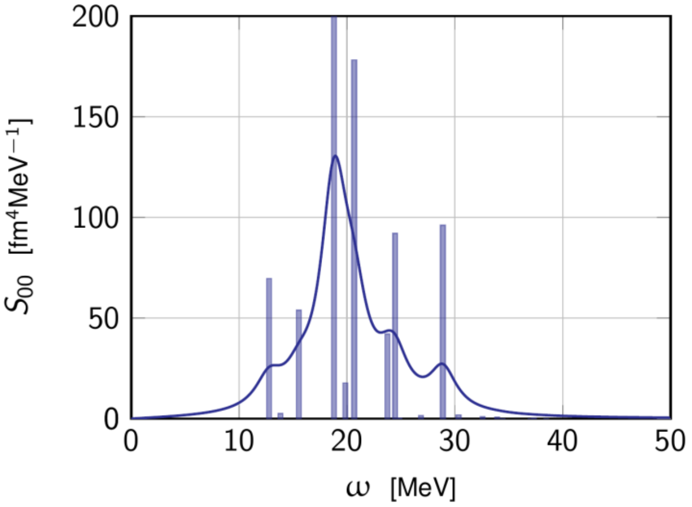

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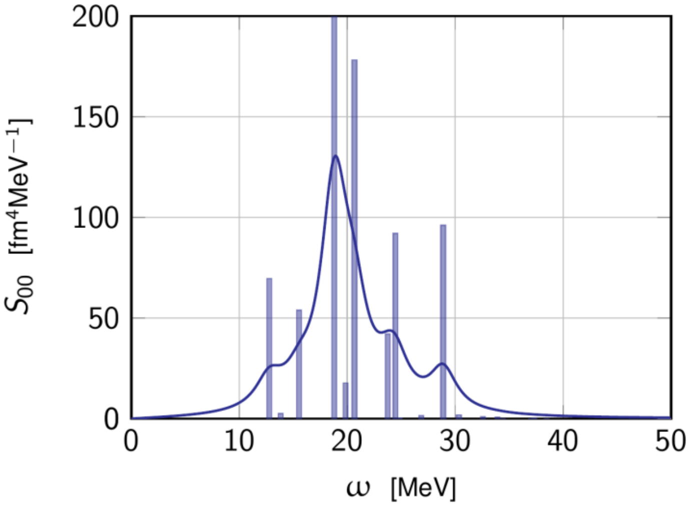
- Related moments

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



[Bohigas et al., 1979]

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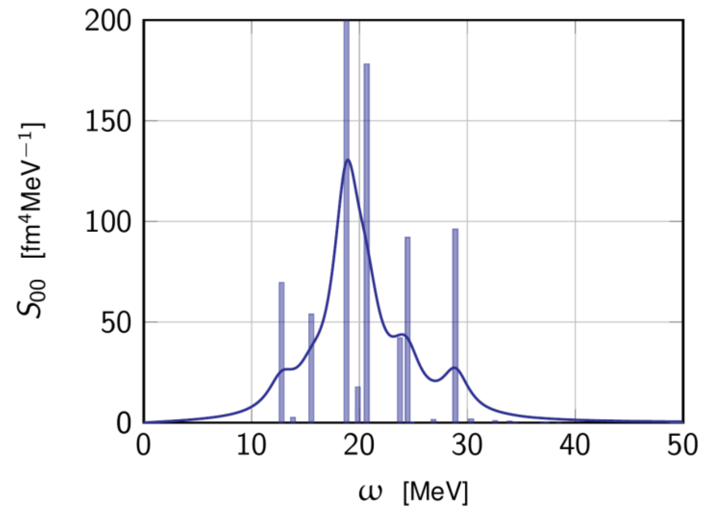
→ Must know excited states



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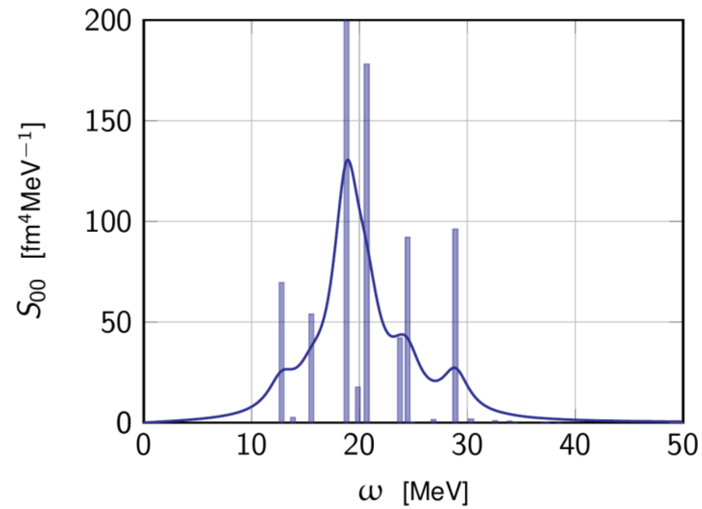

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$$\equiv \langle \Psi_0 | \check{M}_k(i,j) | \Psi_0 \rangle \longrightarrow \text{Ground state only}$$

[Bohigas et al., 1979]

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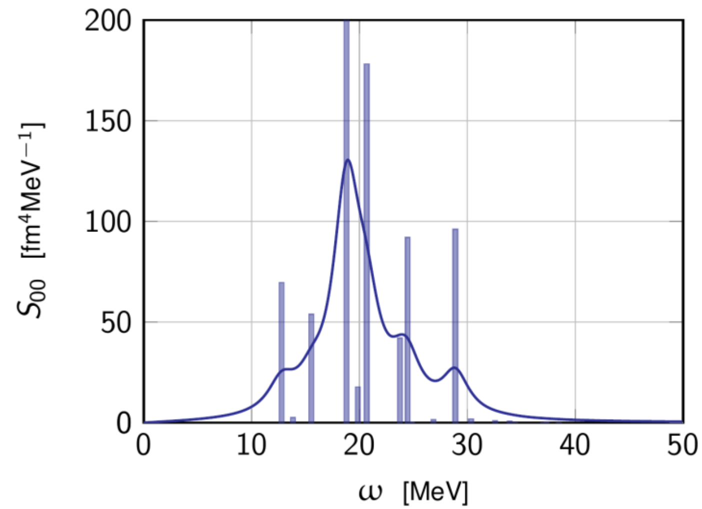

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$$\equiv \langle \Psi_0 | \breve{M}_k(i,j) | \Psi_0 \rangle$$ → Ground state only [Bohigas et al., 1979]

Complexity is shifted to the operator structure

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

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

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

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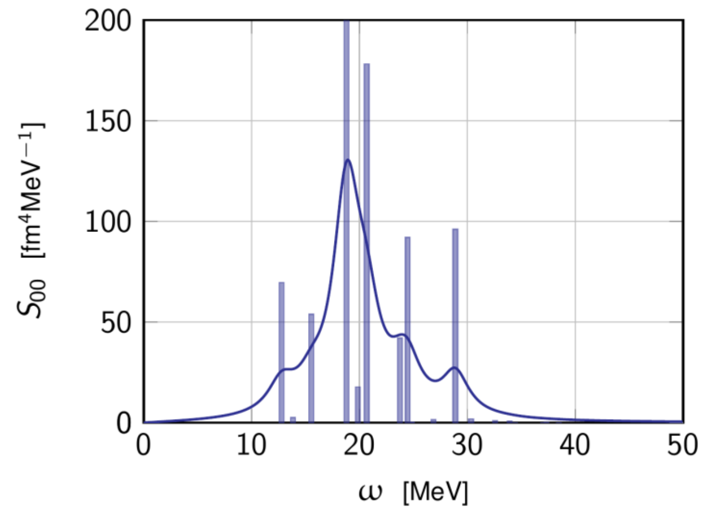
  - Energy difference: position of peaks



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[Bohigas et al., 1979]

Complexity is shifted to the operator structure

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Encode the main physical features of the strength

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

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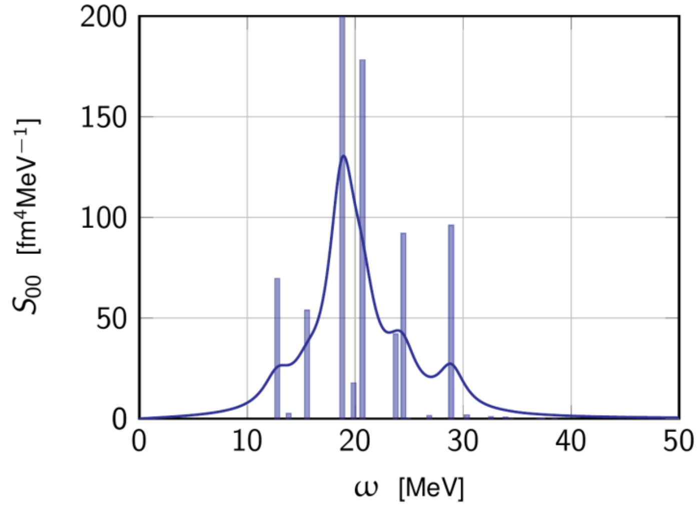

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First comparison ever of the two approaches !

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

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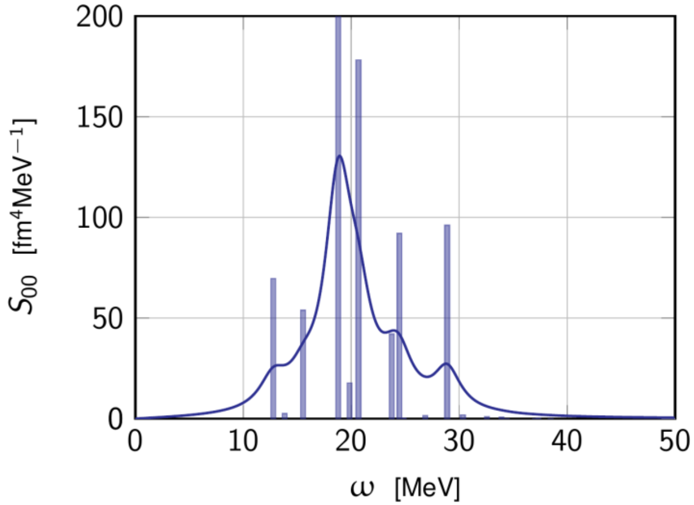

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^{16}O

	m0	m1	m1/m0
QRPA	358,2	8532	23,82
QFAM	358,2	8532	23,82
PGCM sum	356,4	8105	22,74
PGCM gs	380,6	8543	22,45

Benchmark

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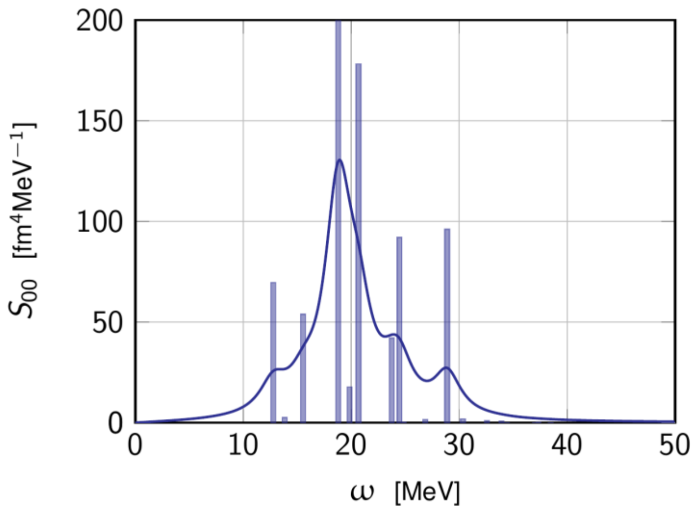

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Benchmark

^{24}Mg

	m0	m1	m1/m0
QFAM	852,4	17.441	20,46
PGCM sum	880,0	17.049	19,37
PGCM gs	960,1	17.760	18,50

Moments and Sum Rules

Sum rules are important for the extraction of experimental data **(MDA)**

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Many-body operators

- Exact up to m_1 $\quad H = H^{[1]} + H^{[2]}$
- Different approximations $\quad H \approx H^{[1]}$

Outline

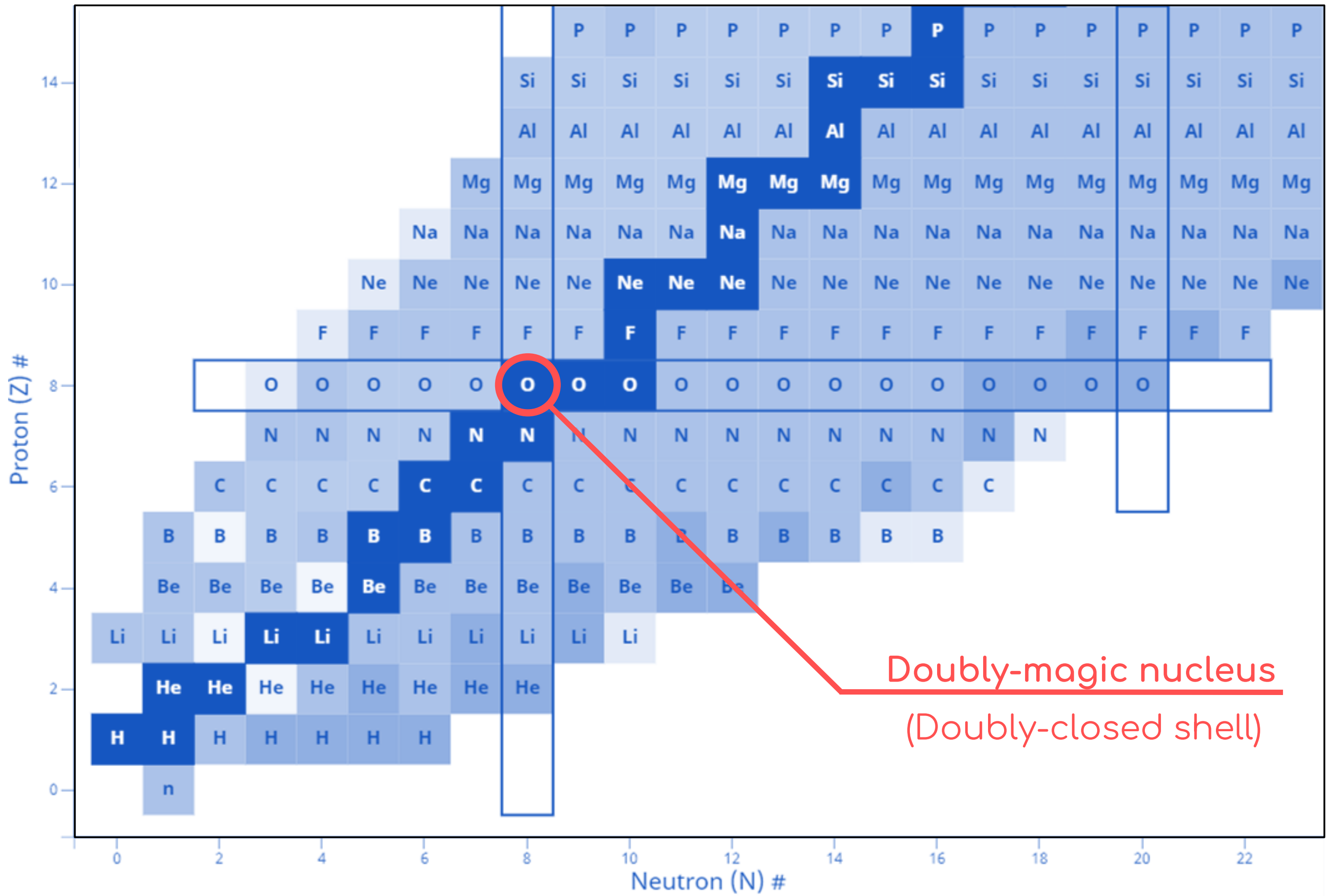
- Introduction
- Formalism
- **Preliminary results**
- Conclusions

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
- The PGCM wavefunction explores the β_2 and r^2 collective coordinates (quadrupolar coupling)

Benchmarking ^{16}O

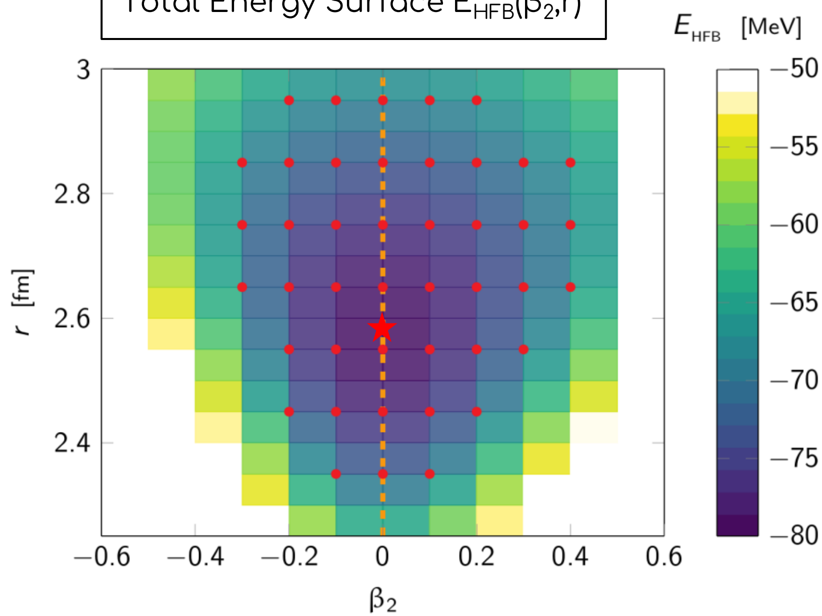


Benchmarking ^{16}O

Difficulty

☐ Benchmark on existing spherical QRPA code

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



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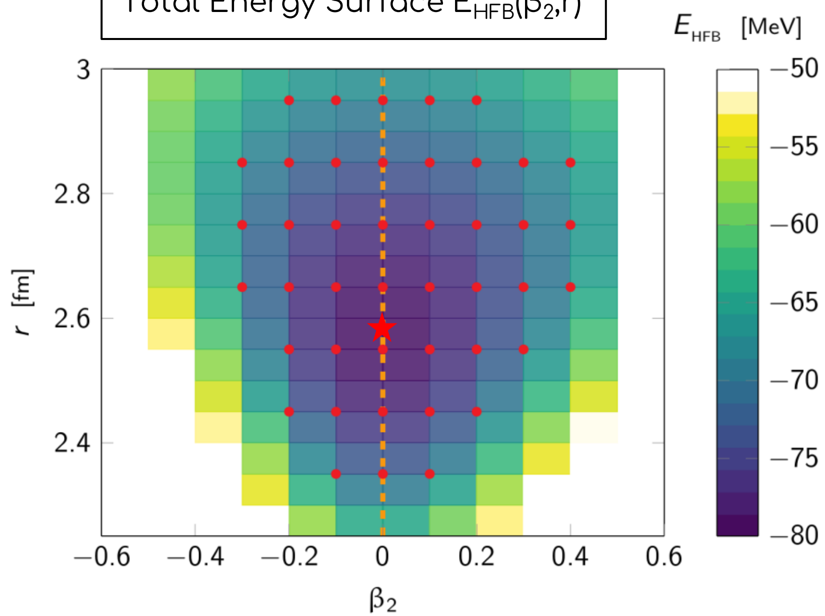

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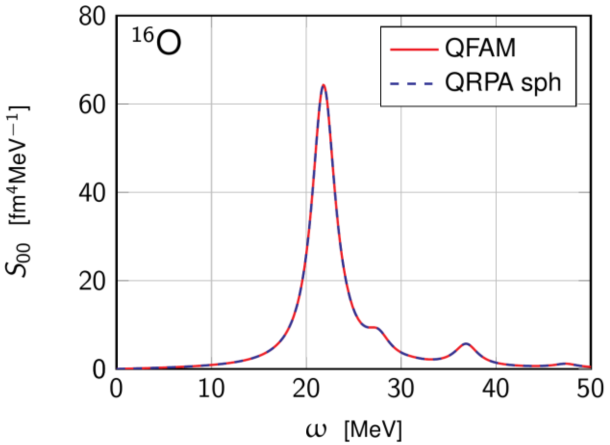

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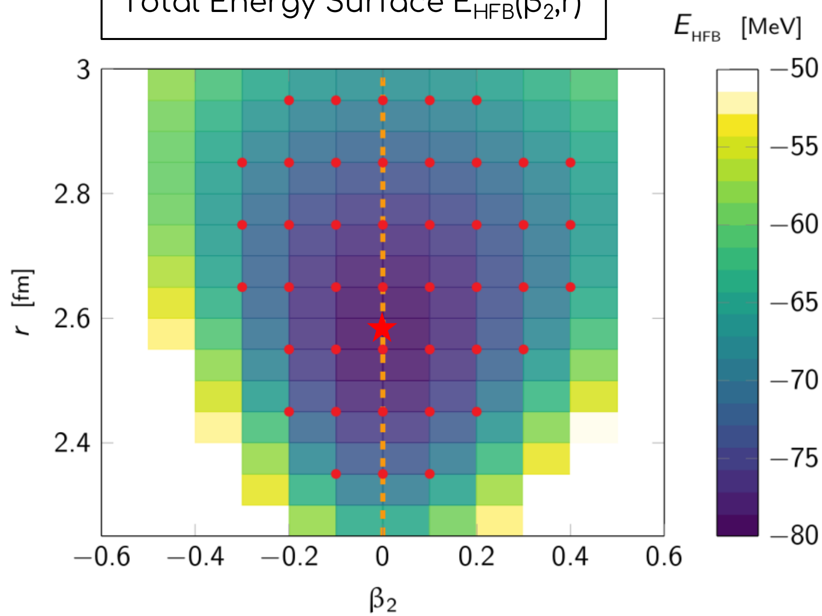

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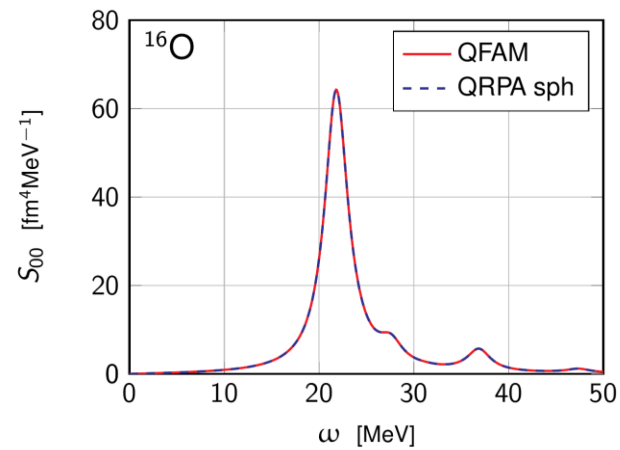

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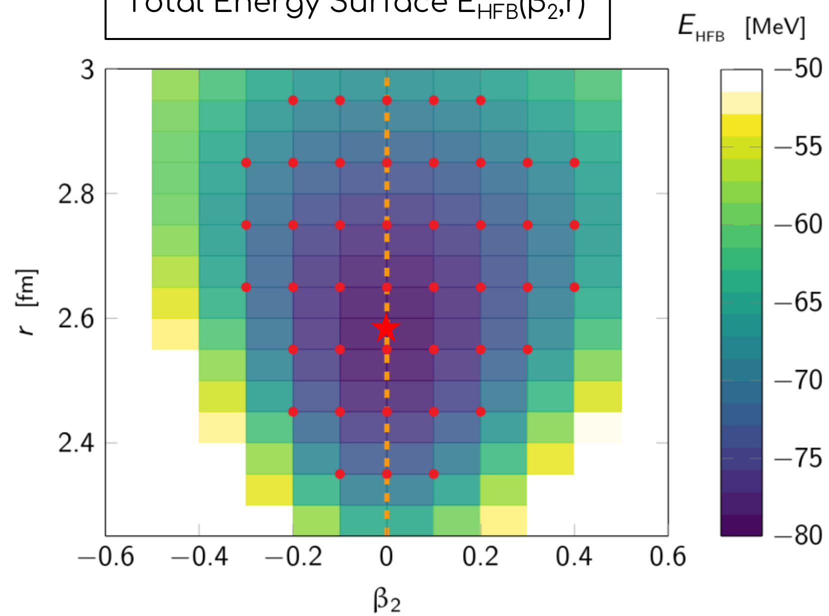

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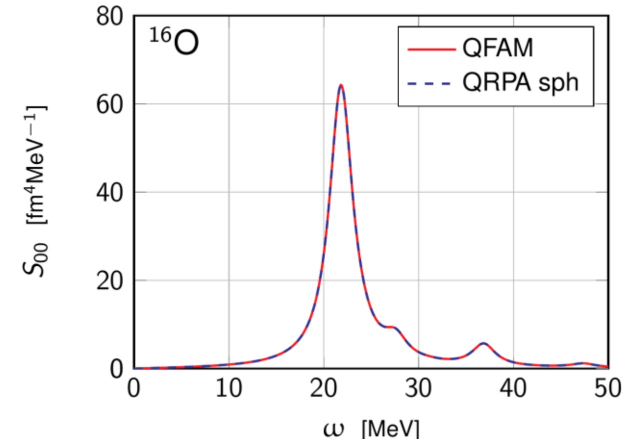

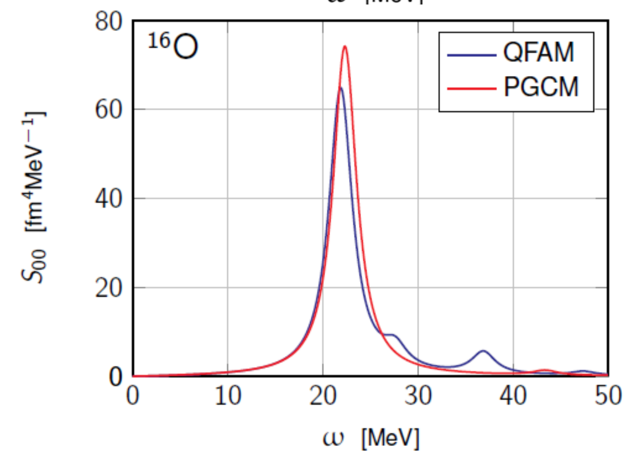

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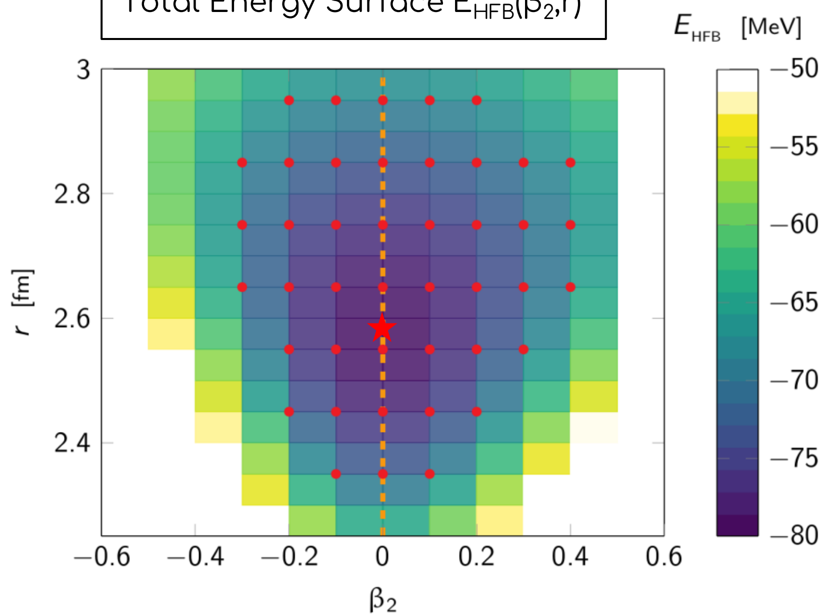

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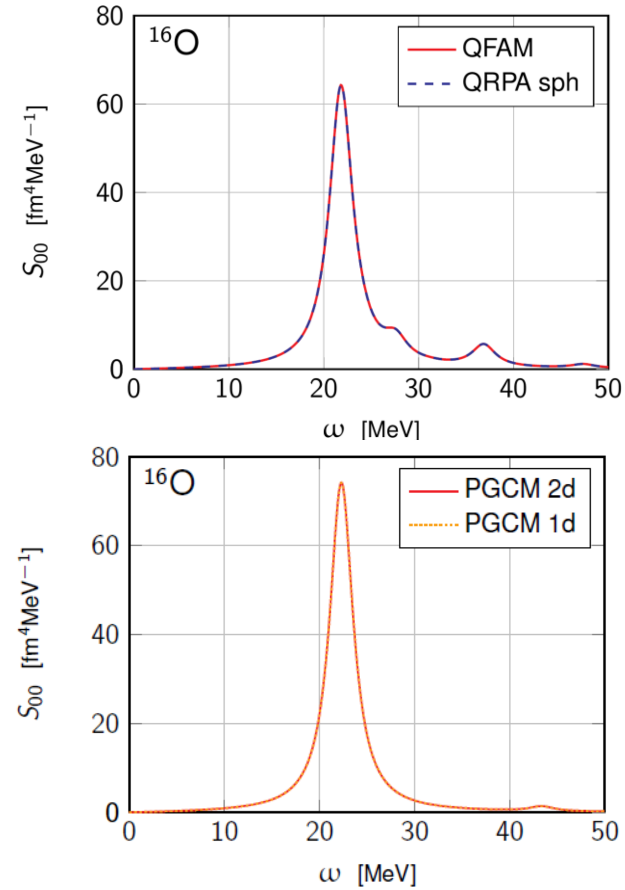

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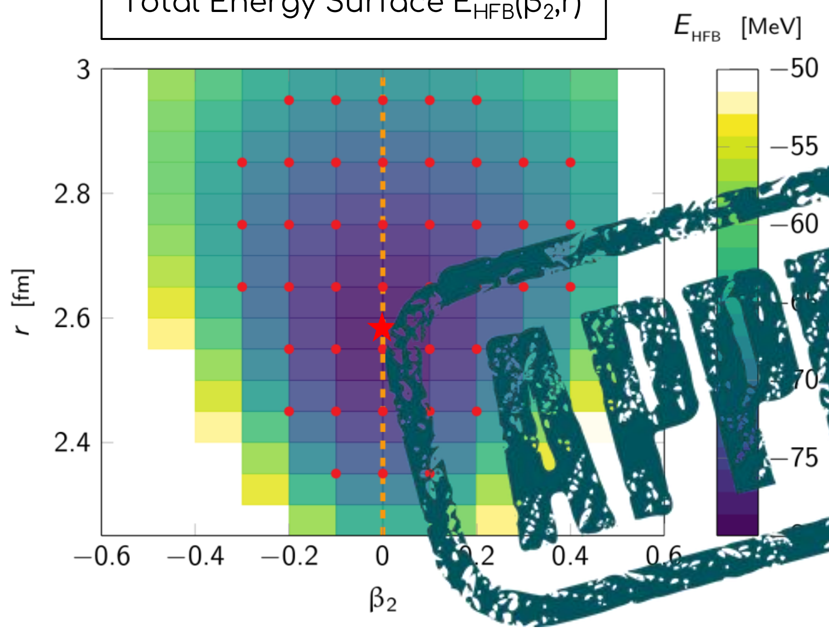

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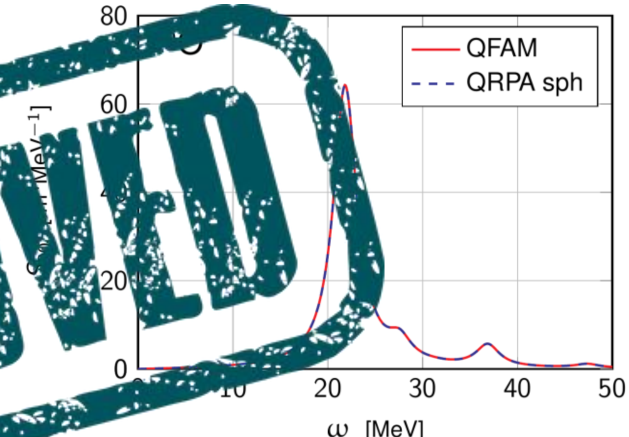

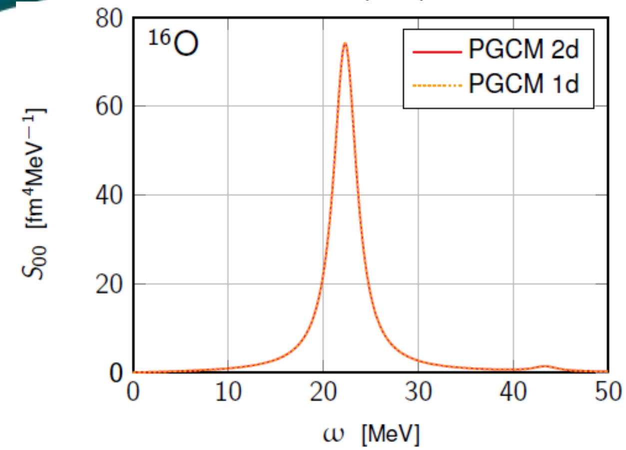

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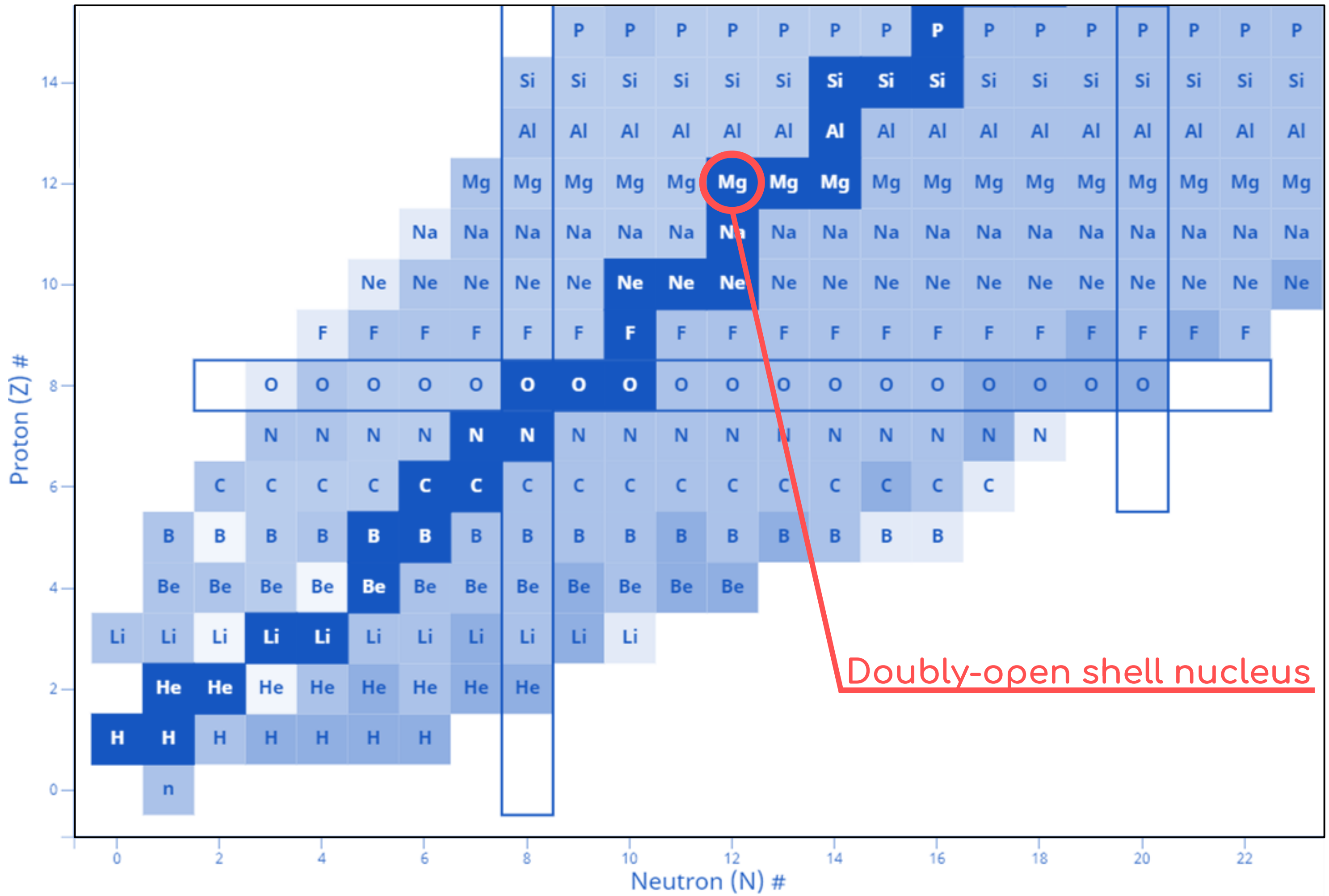
Deformation effects in ^{24}Mg



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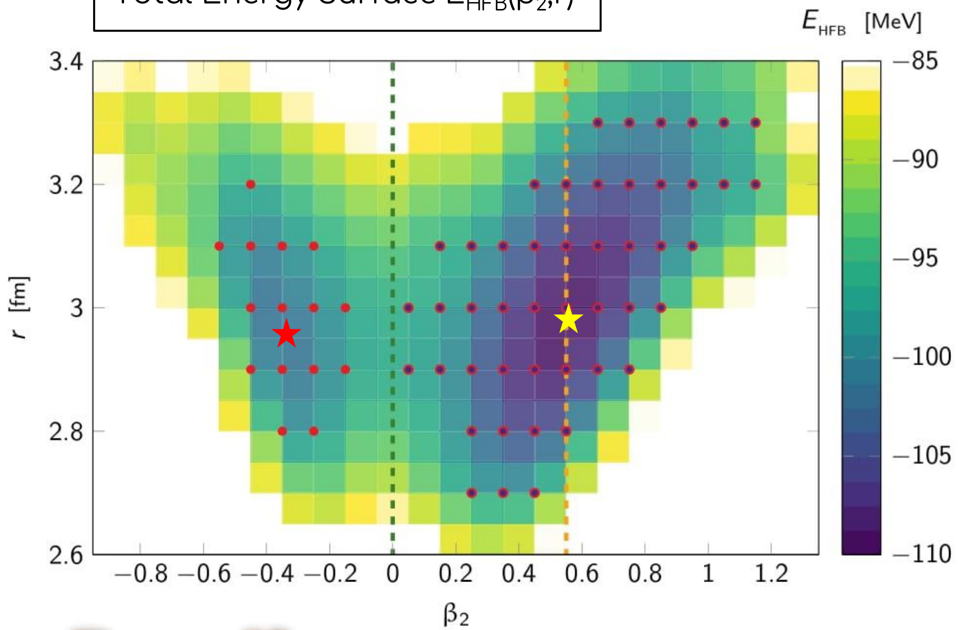

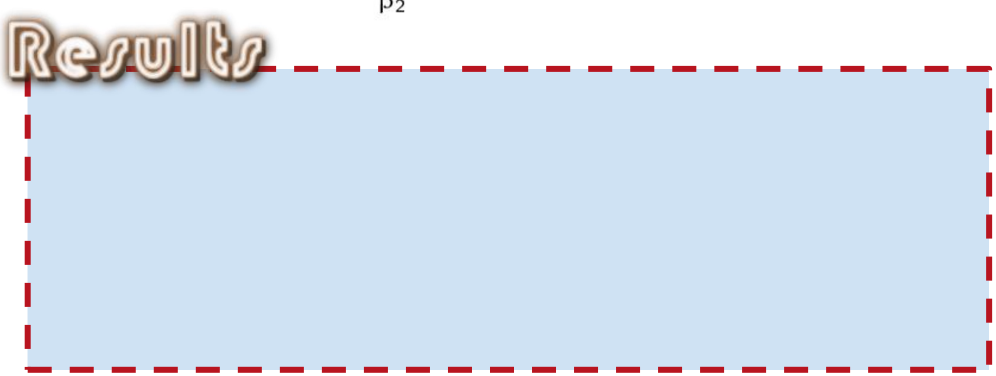

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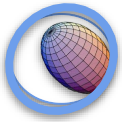

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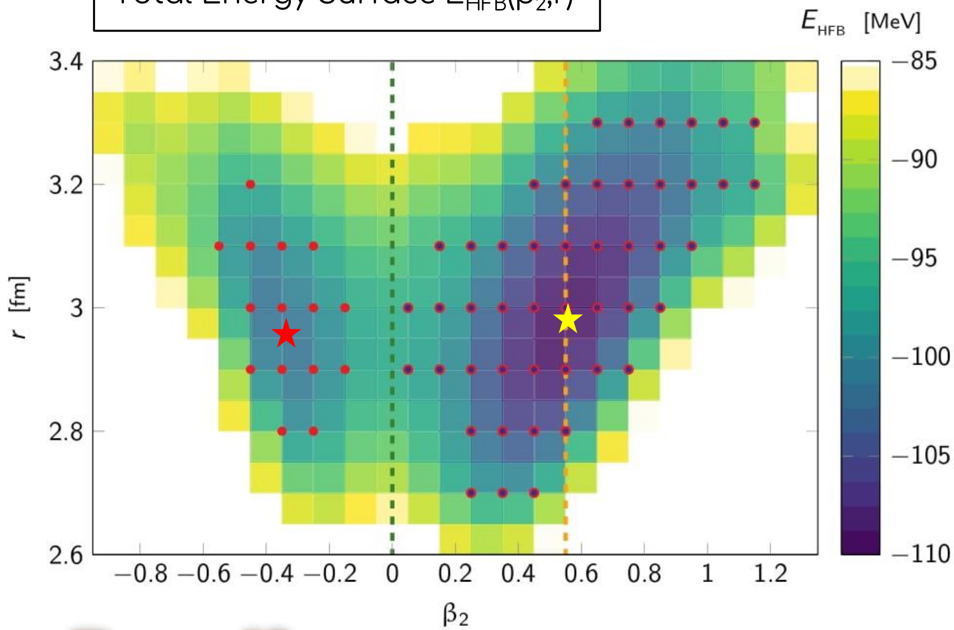

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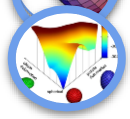

Shape coexistence ? [1]

(1) [Dowie et al., 2020]

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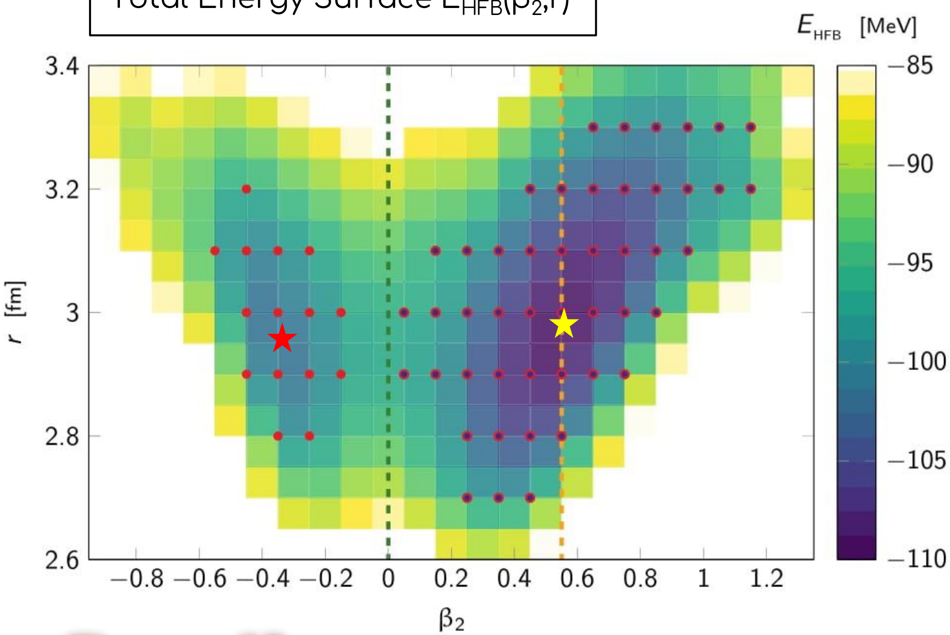

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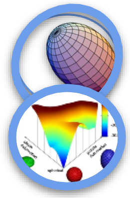

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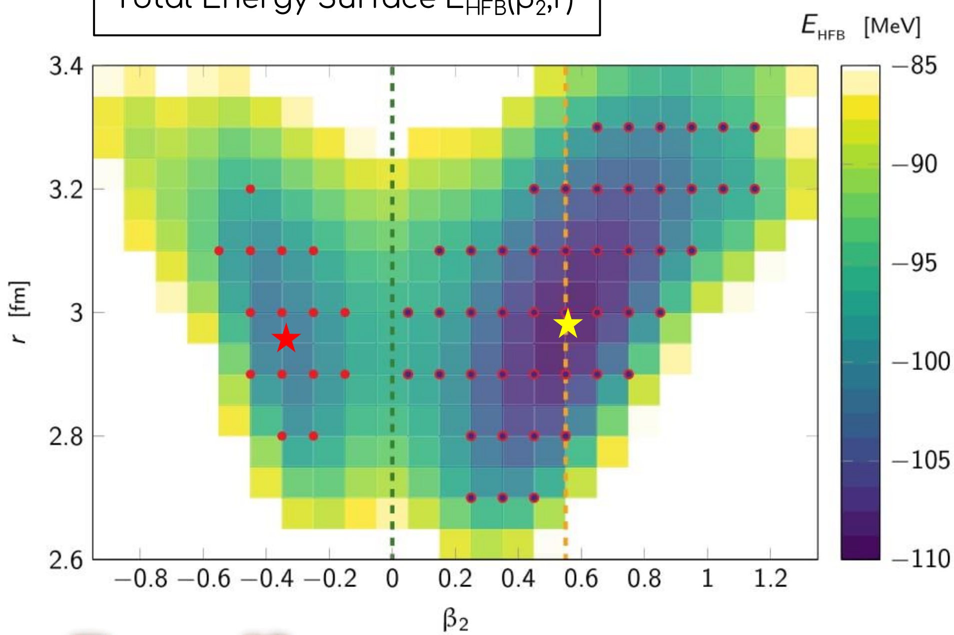

Results

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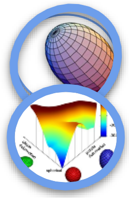

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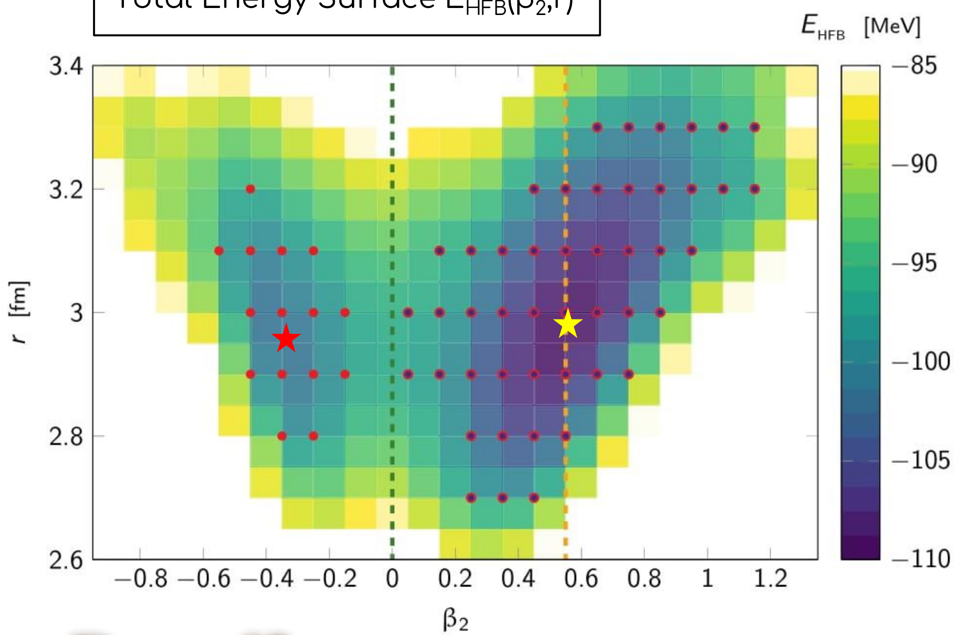

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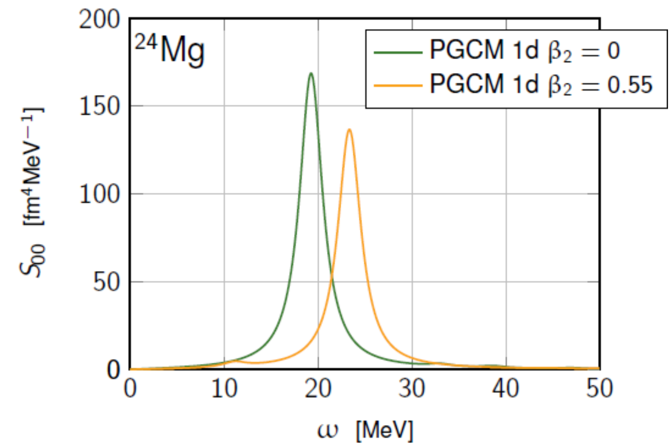

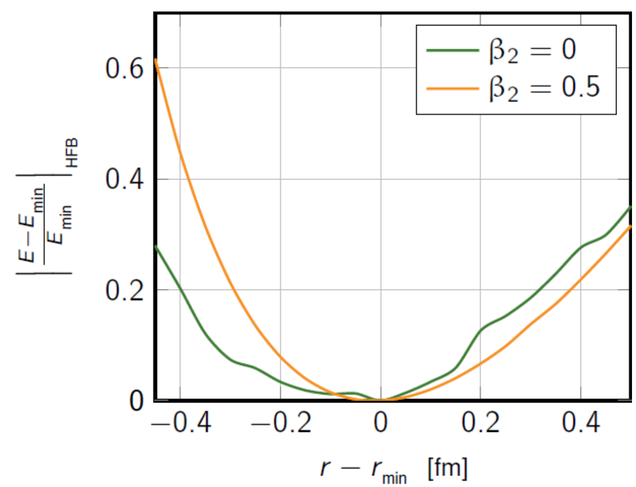

Results

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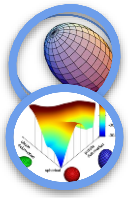
- Static deformation shift up single peak

Deformation effects in ^{24}Mg

Difficulty



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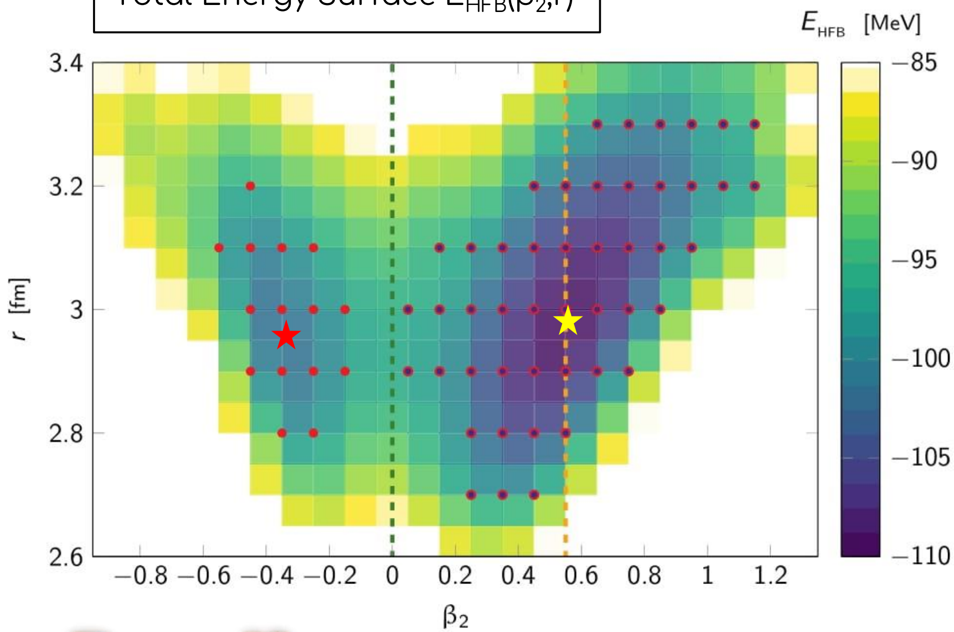

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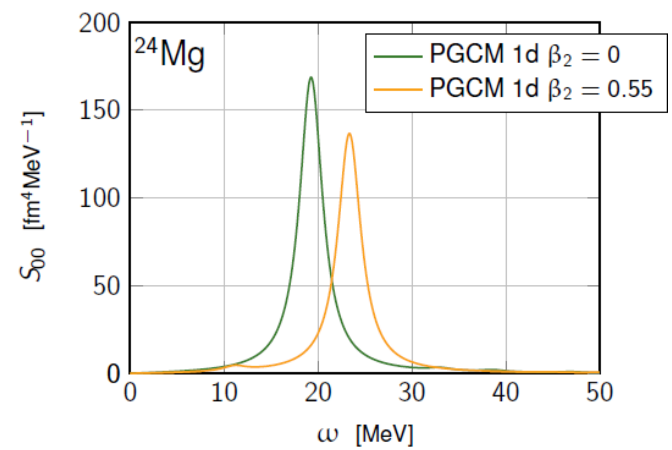

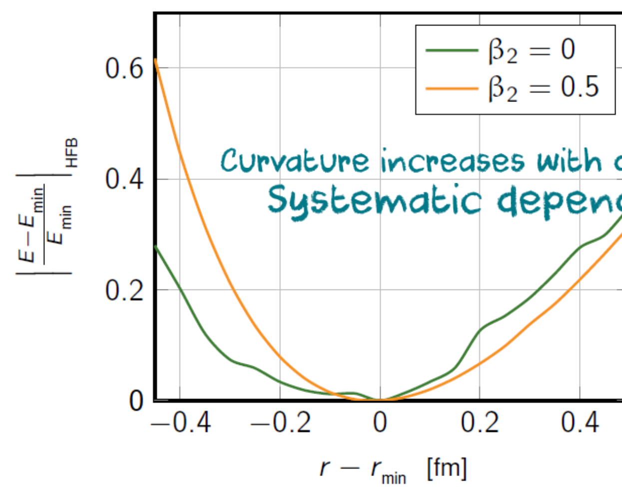

Curvature increases with deformation

Systematic dependency ?

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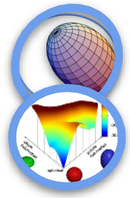

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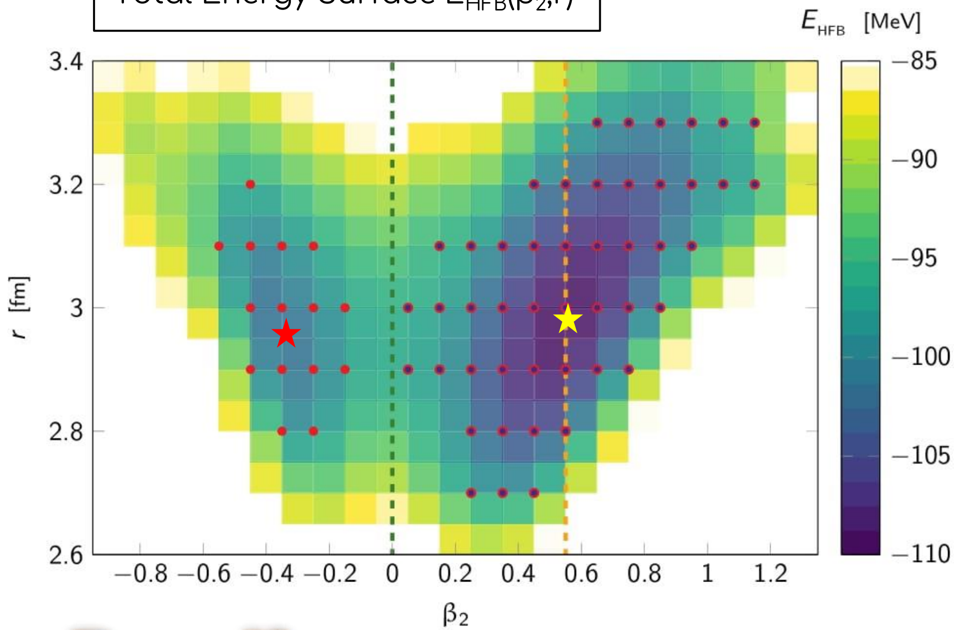

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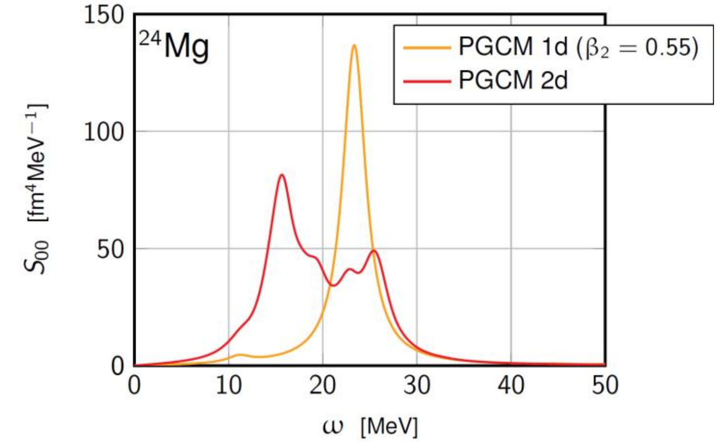
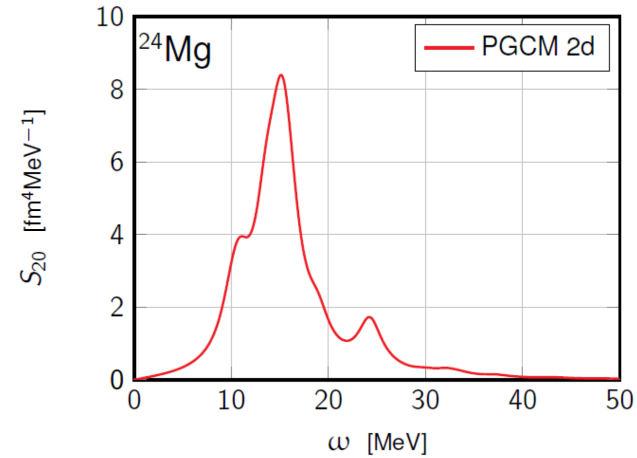


K=0 Quadrupole Strength



Results

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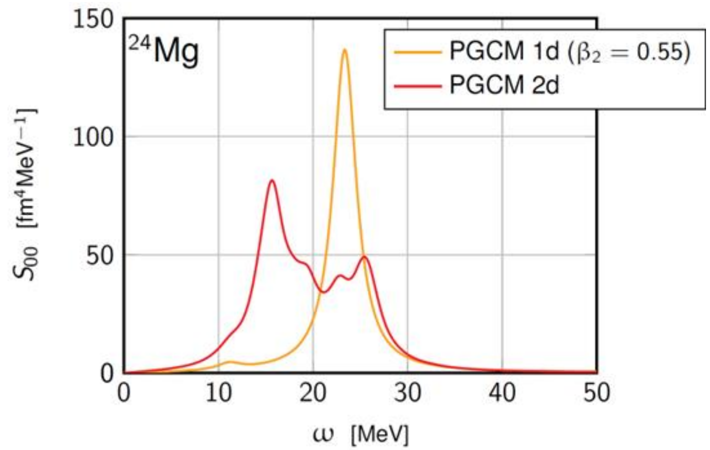
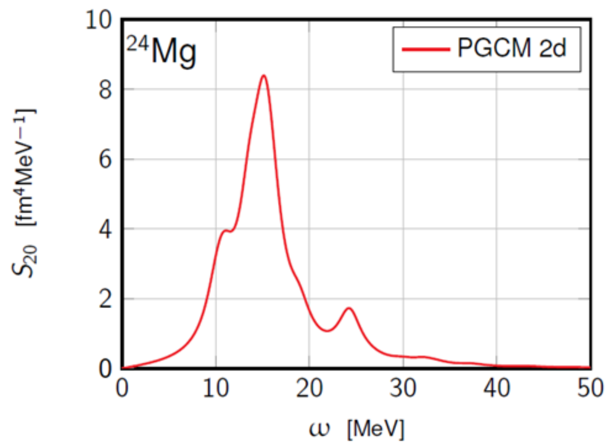
- Static deformation shift up single peak
- Coupling to GQR generates splitting
  - × High peak = shifted “spherical” breathing mode
  - × Low peak = induced by coupling to GQR (K=0)

Deformation effects in ^{24}Mg

Monopole Strength



K=0 Quadrupole Strength



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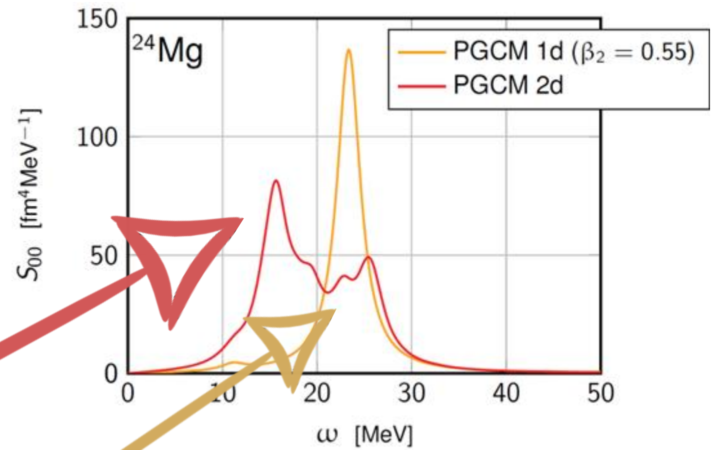
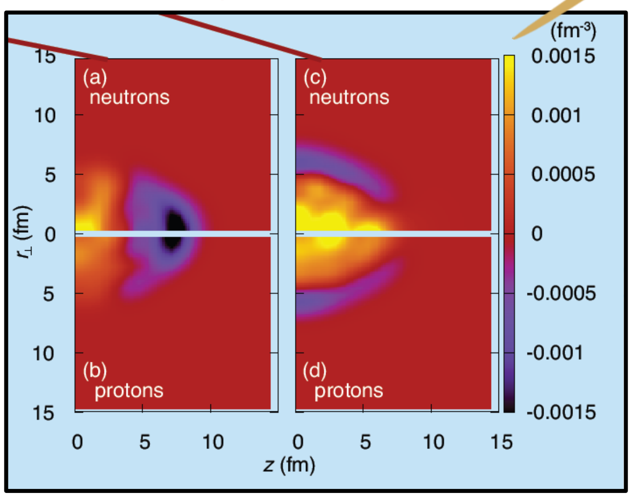


[From K. Yoshida's talk]

Intrinsic QRPA transition densities



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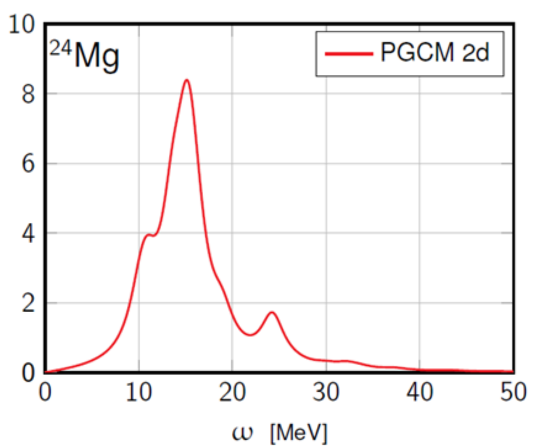
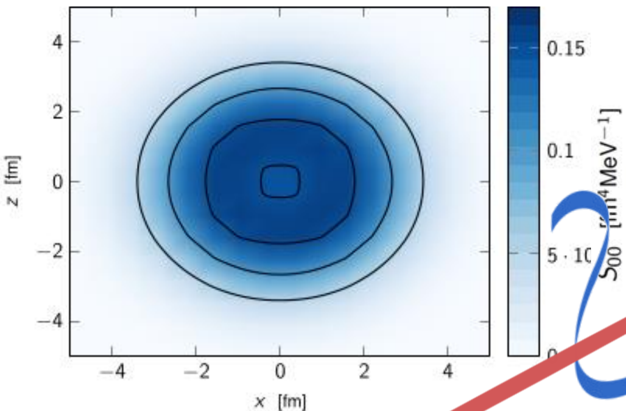


Deformation effects in ^{24}Mg

Ground-state density



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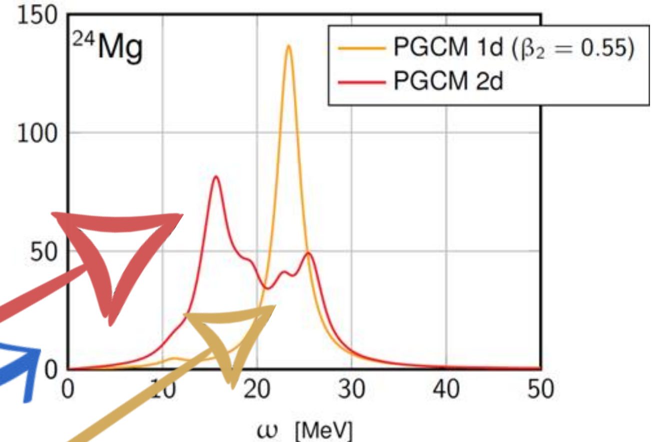

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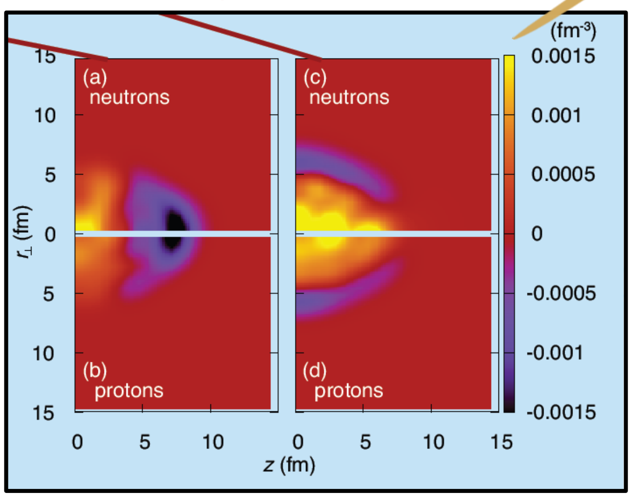

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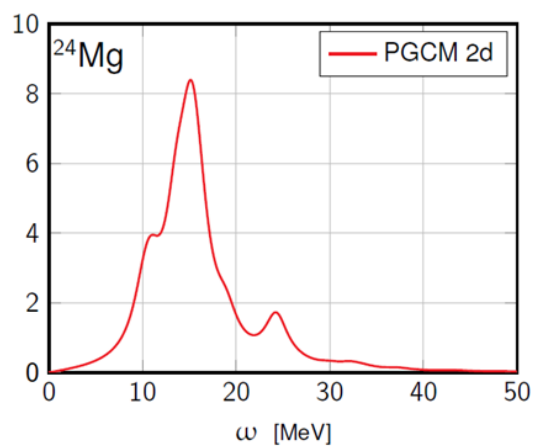

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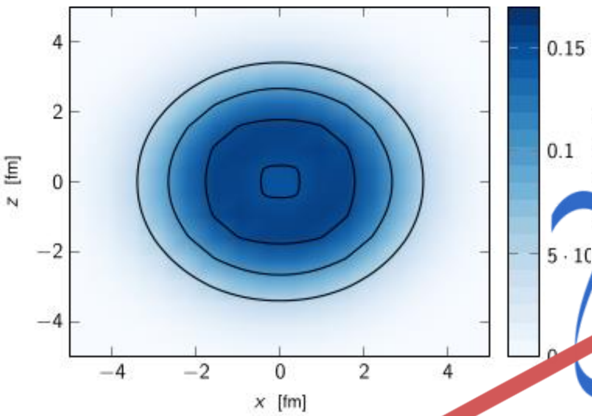

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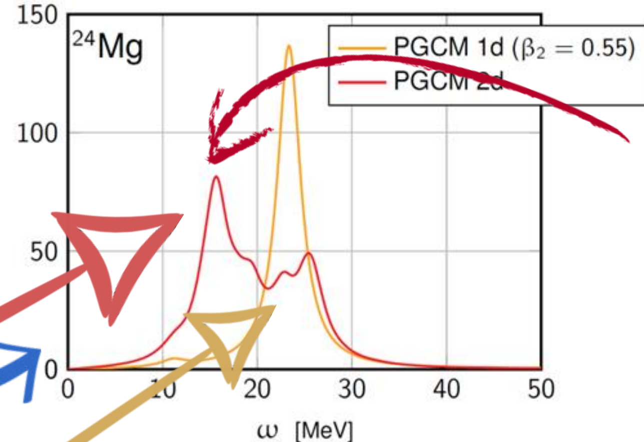
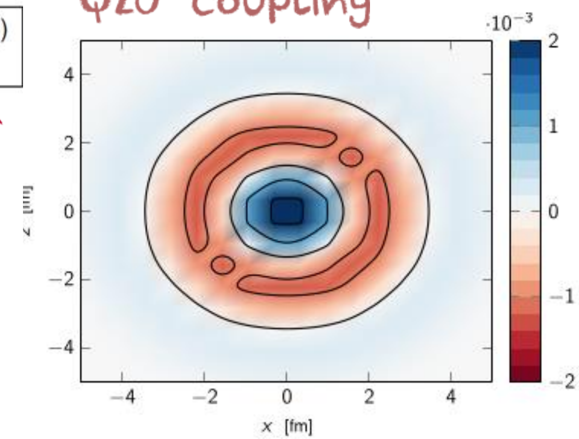


Densities in lab frame

First peak

Q20 coupling



[From K. Yoshida's talk]

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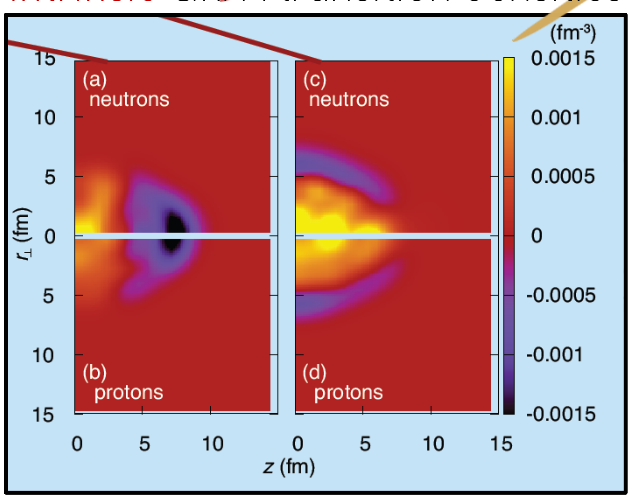

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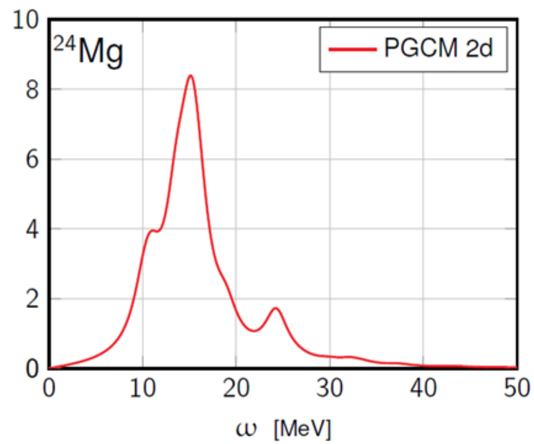

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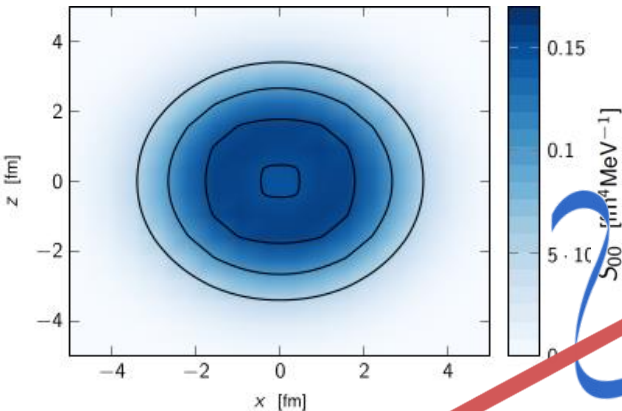

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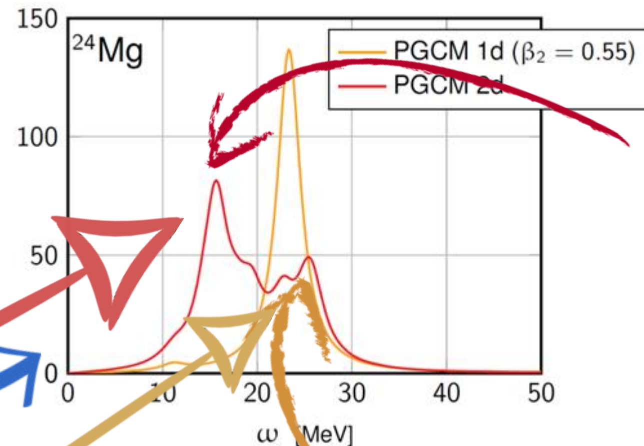

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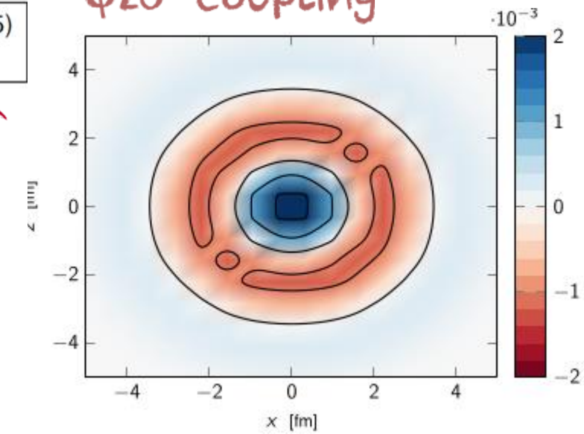

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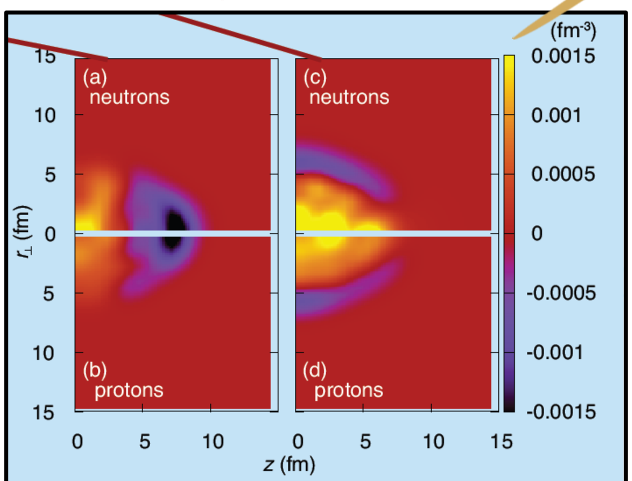

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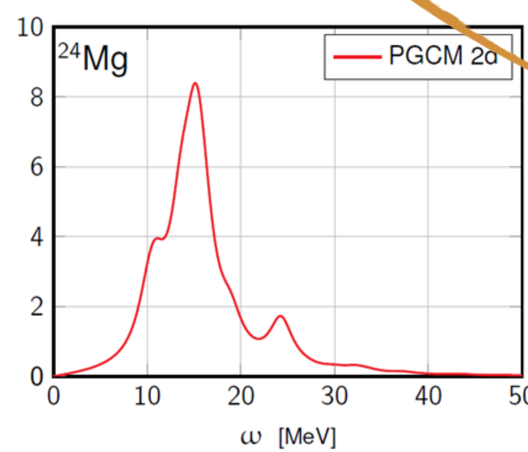
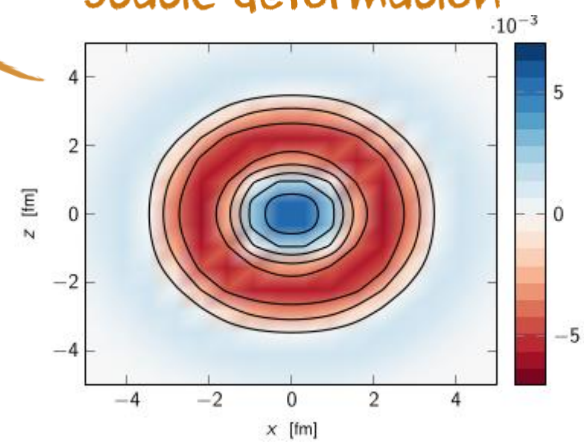
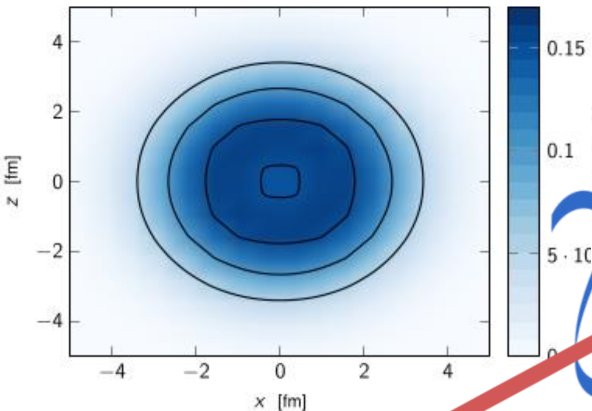


Second peak
Static deformation

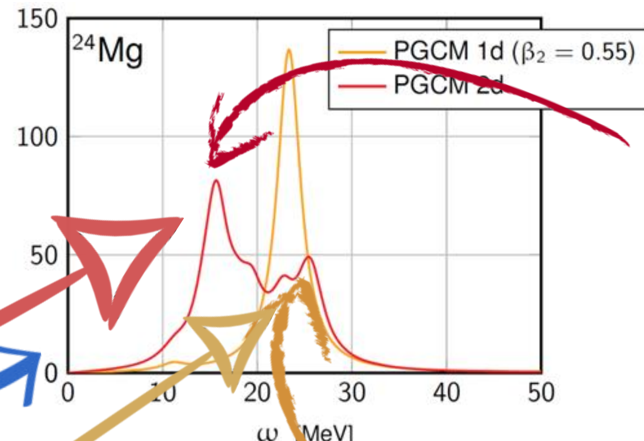


Deformation effects in ^{24}Mg

Ground-state density



Monopole Strength



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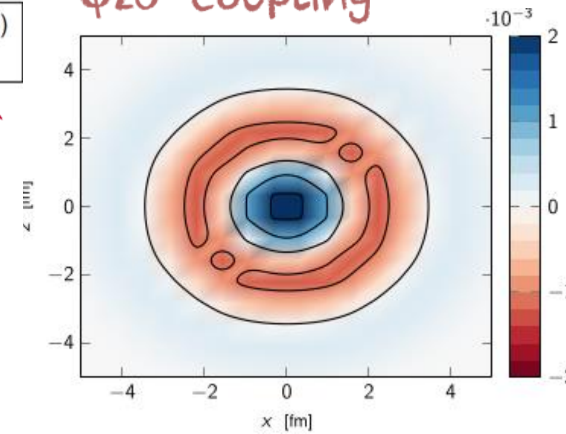

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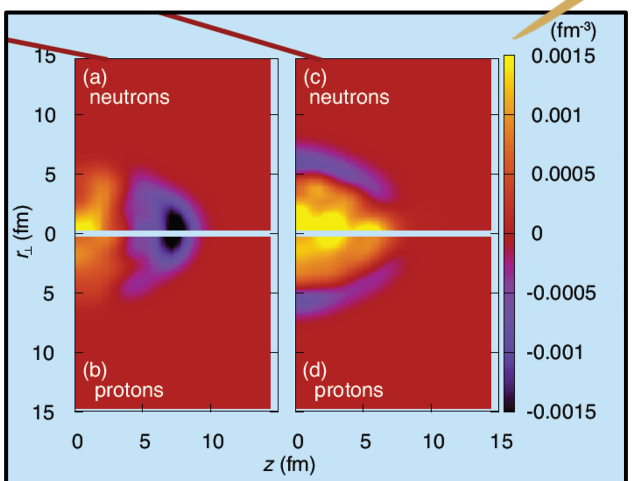

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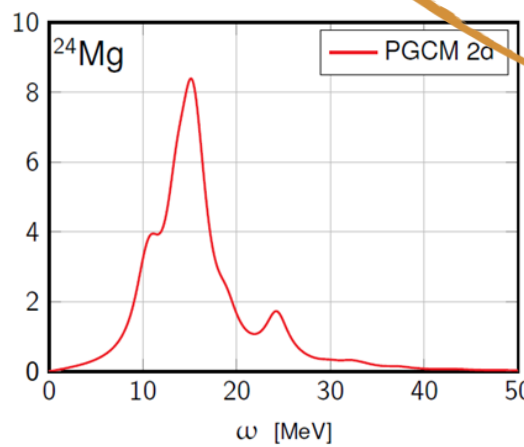
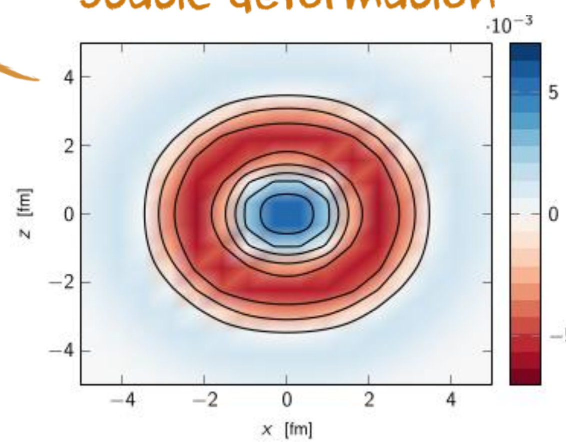


Laboratory frame: any signature ?

Second peak

Static deformation



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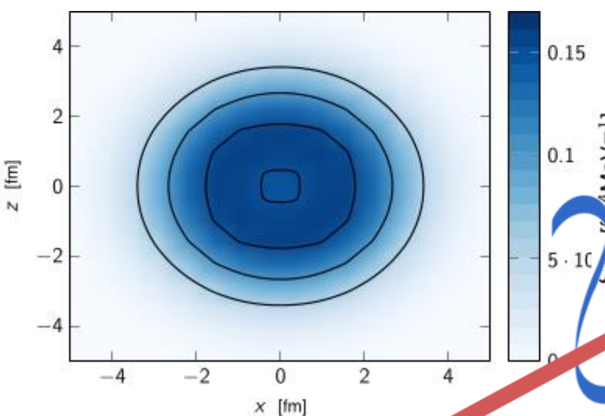

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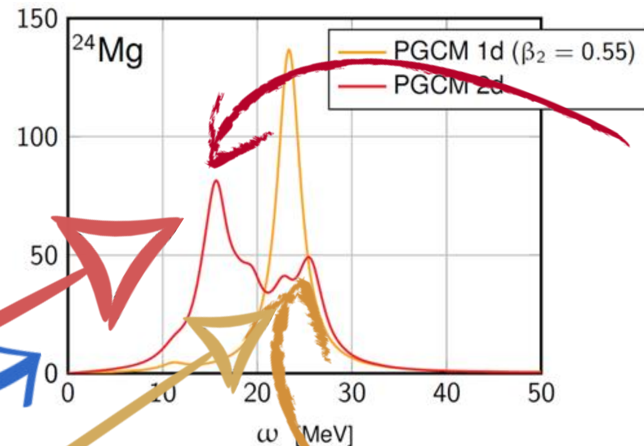

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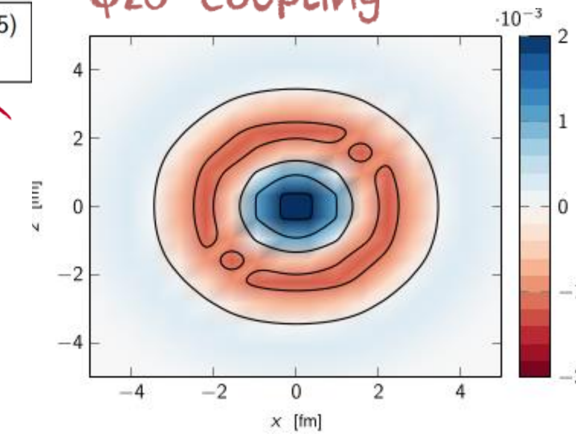

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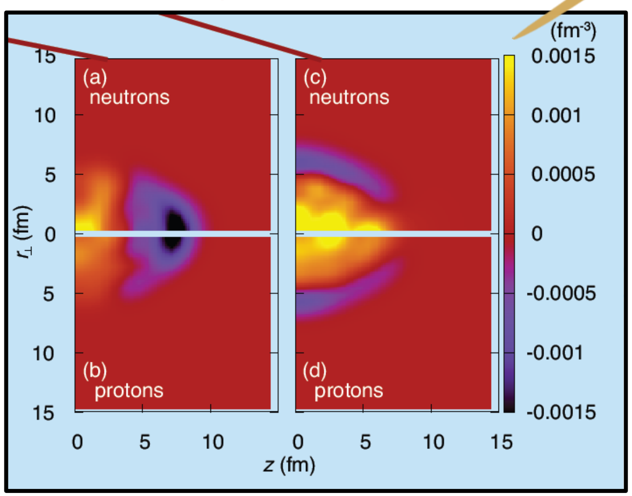

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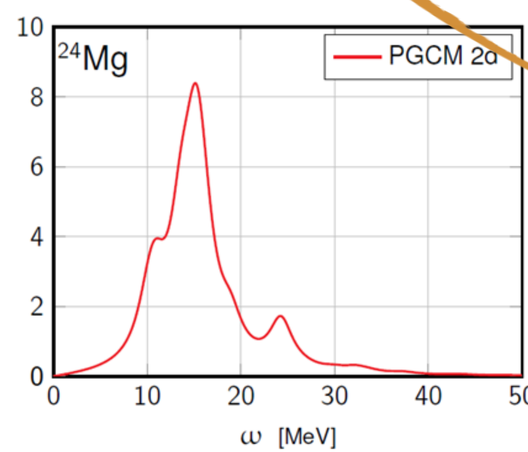

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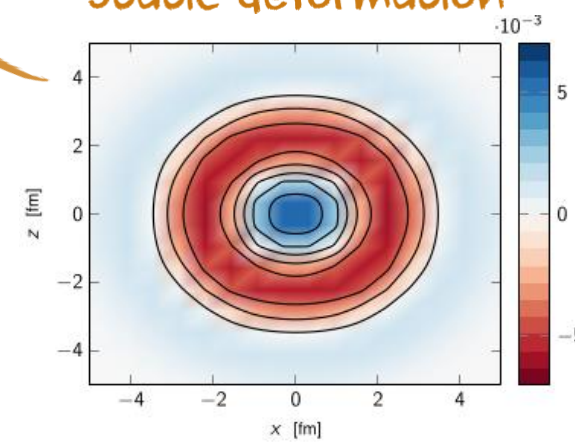
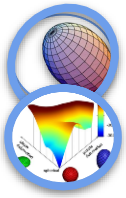


To further investigate !

Deformation effects in ^{24}Mg

Difficulty

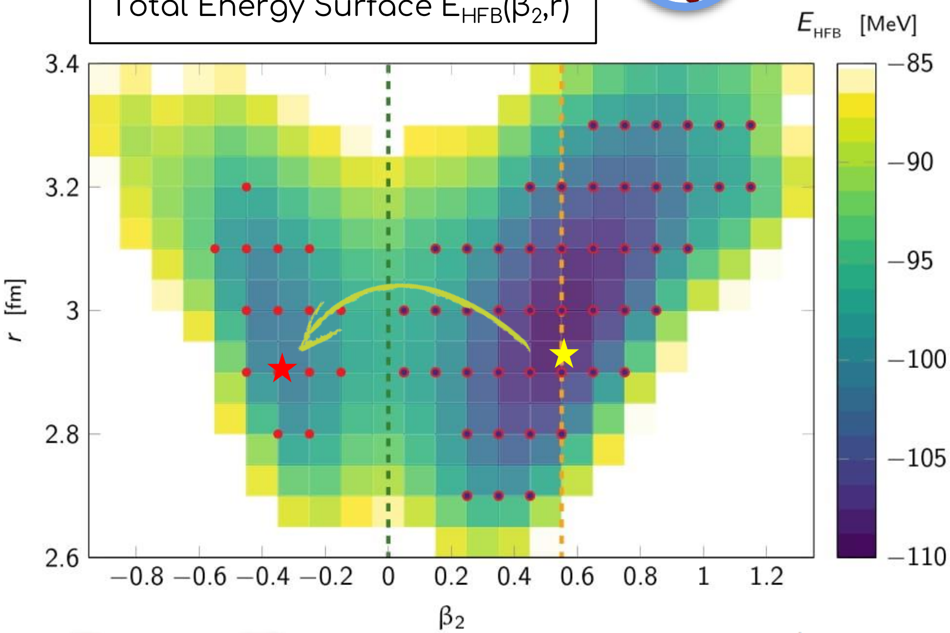


Deformation

Shape coexistence ? [1]

(1) [Dowie et al., 2020]

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



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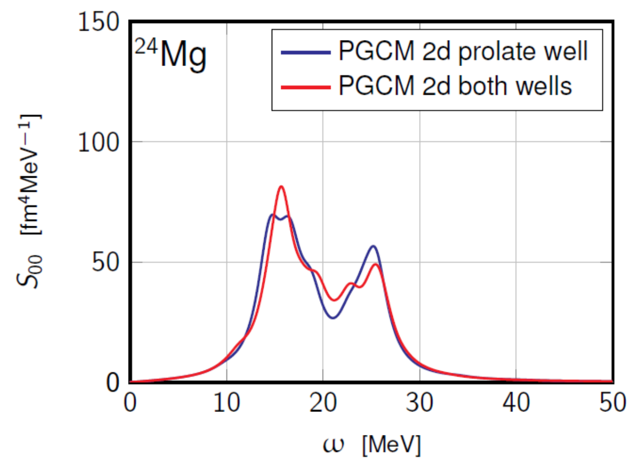

$\Delta E \approx 6.8$ MeV

Results

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  - x No shape mixing effect

Deformation effects in ^{24}Mg

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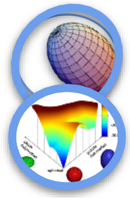

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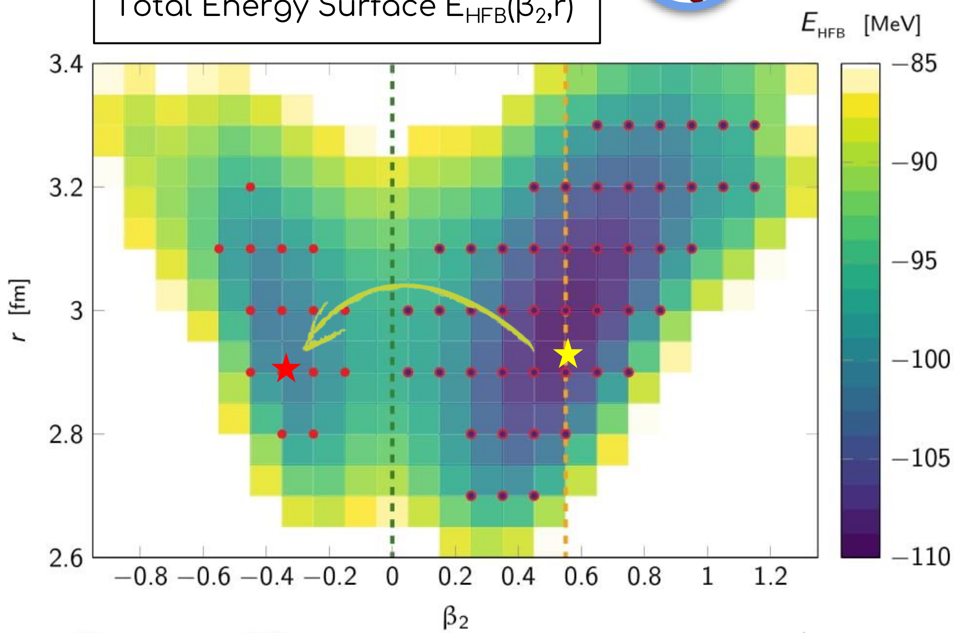

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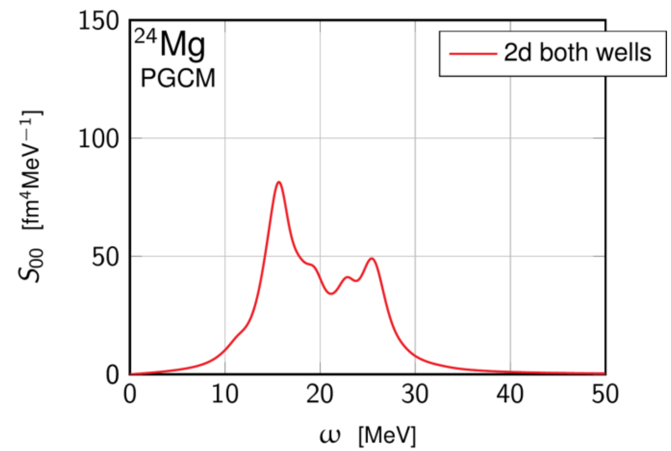

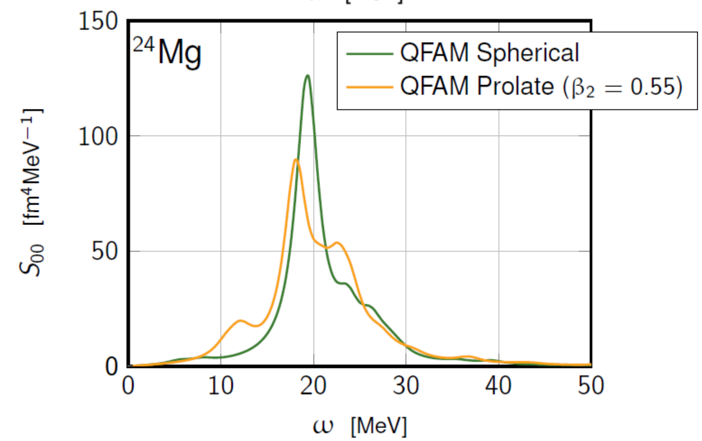

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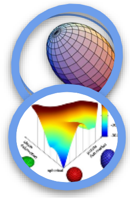

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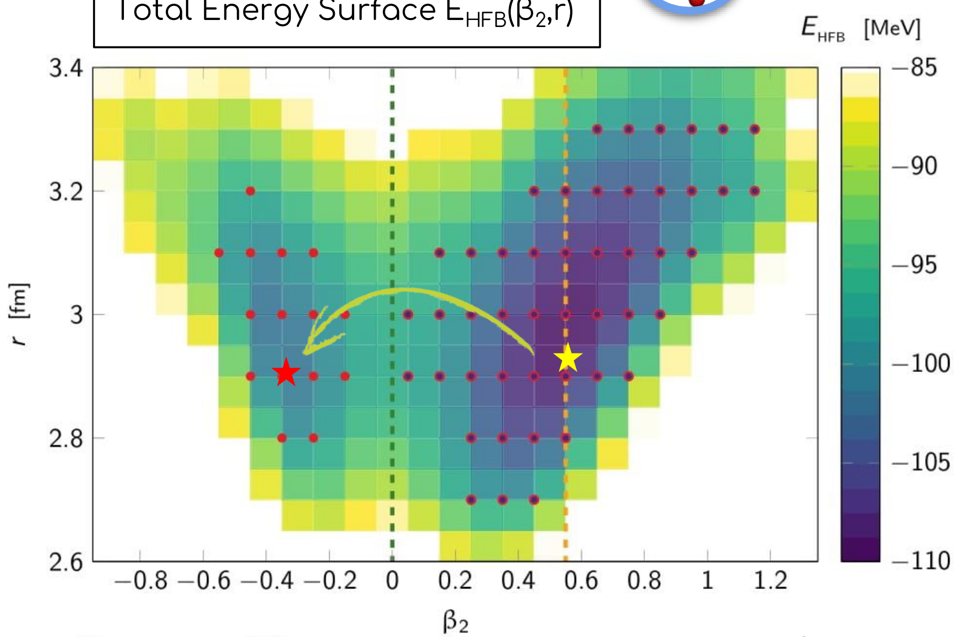

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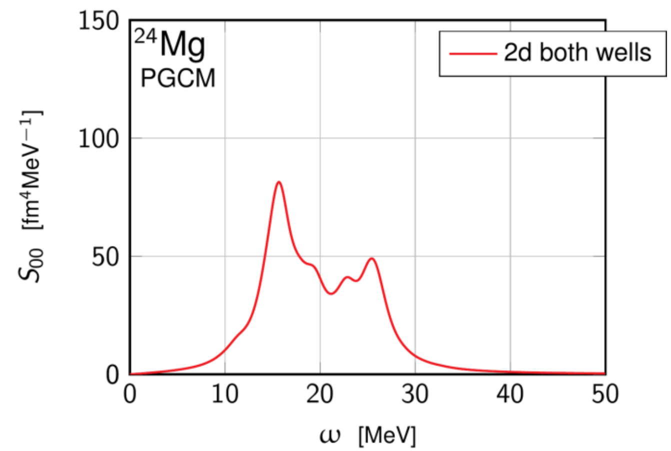

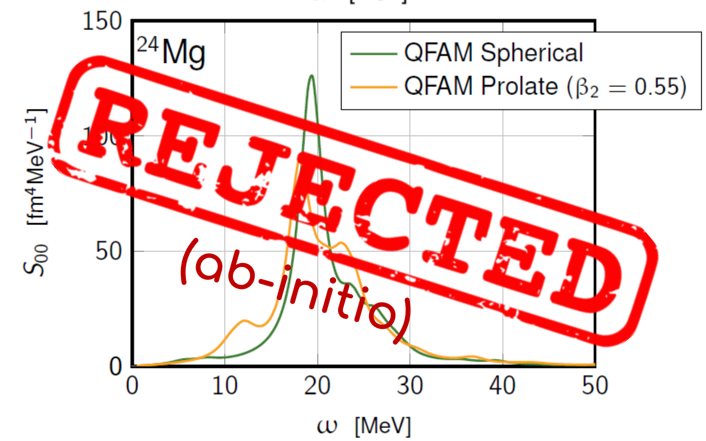

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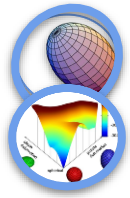

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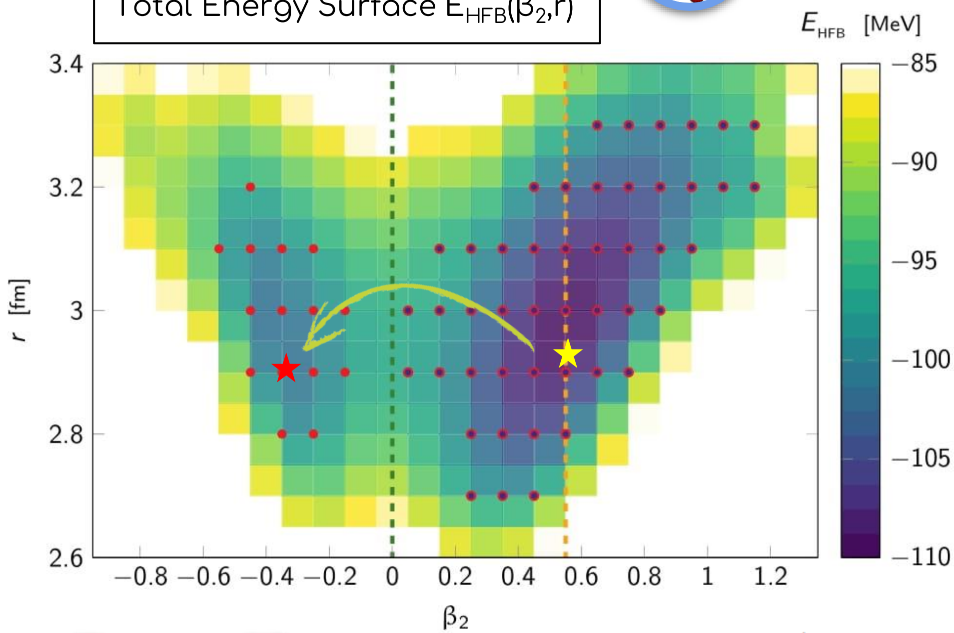

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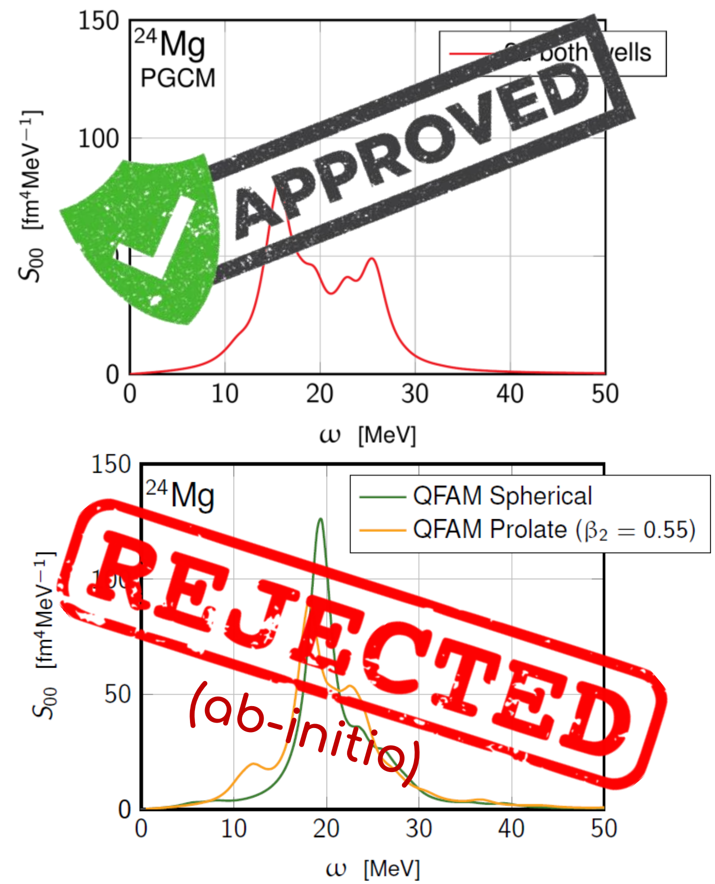

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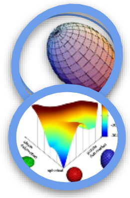

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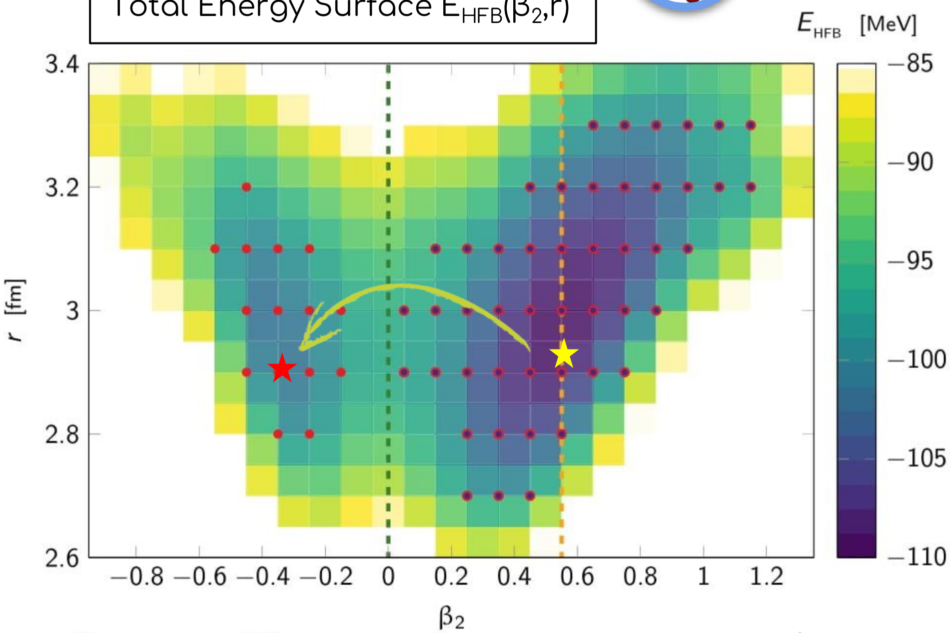

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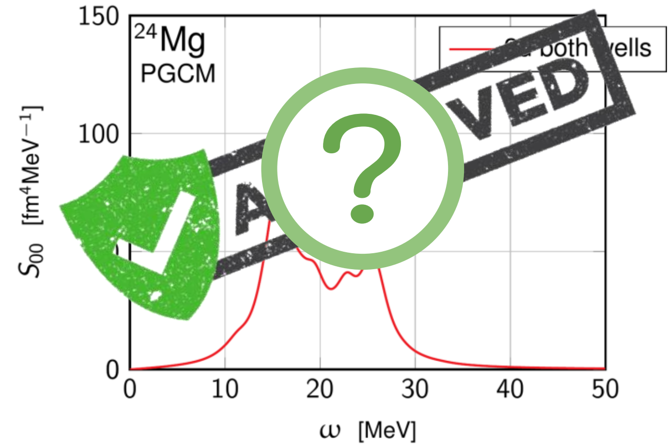

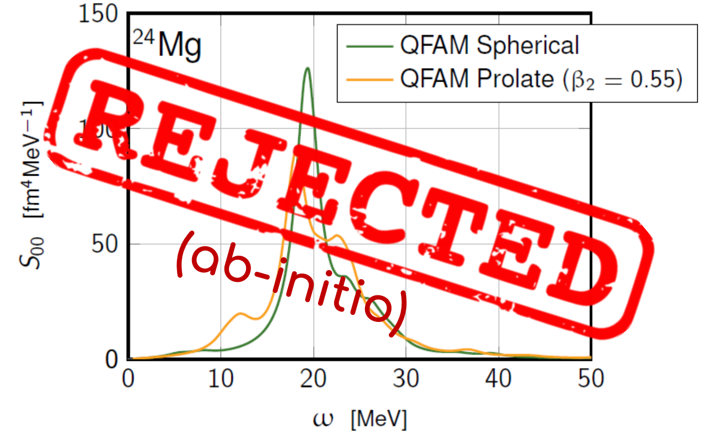

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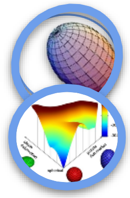

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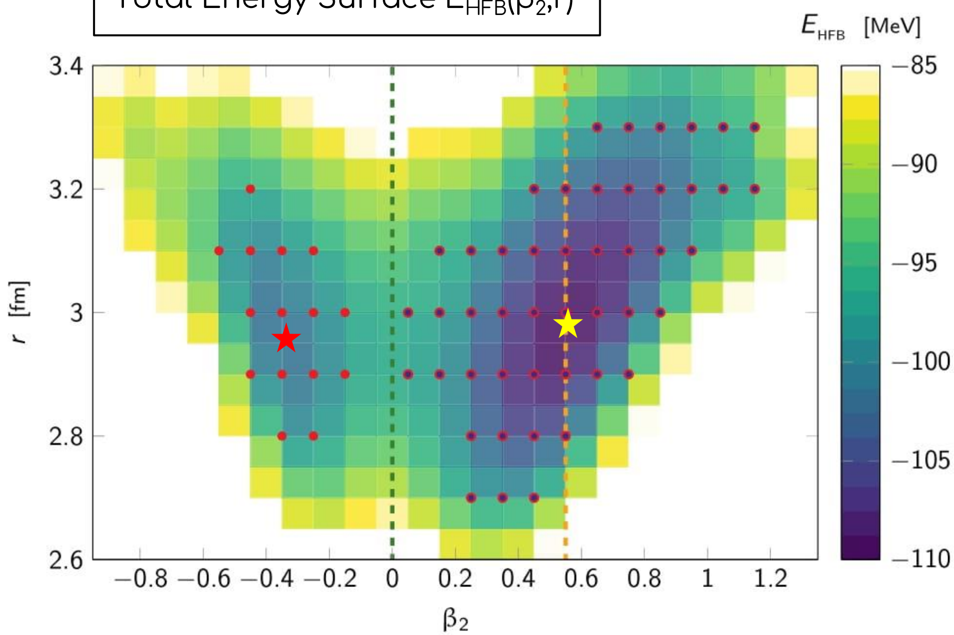

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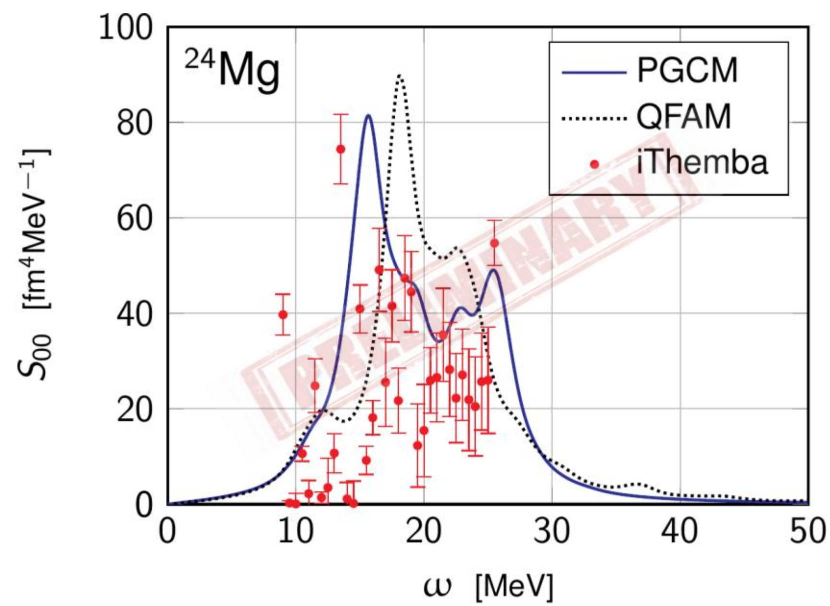
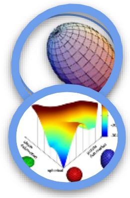


iThemba, Bahini 2021

1. **PGCM superior to QRPA**
2. Experiments **useful** and **promising**
3. Data are **not unambiguous**

Deformation effects in ^{24}Mg

Difficulty



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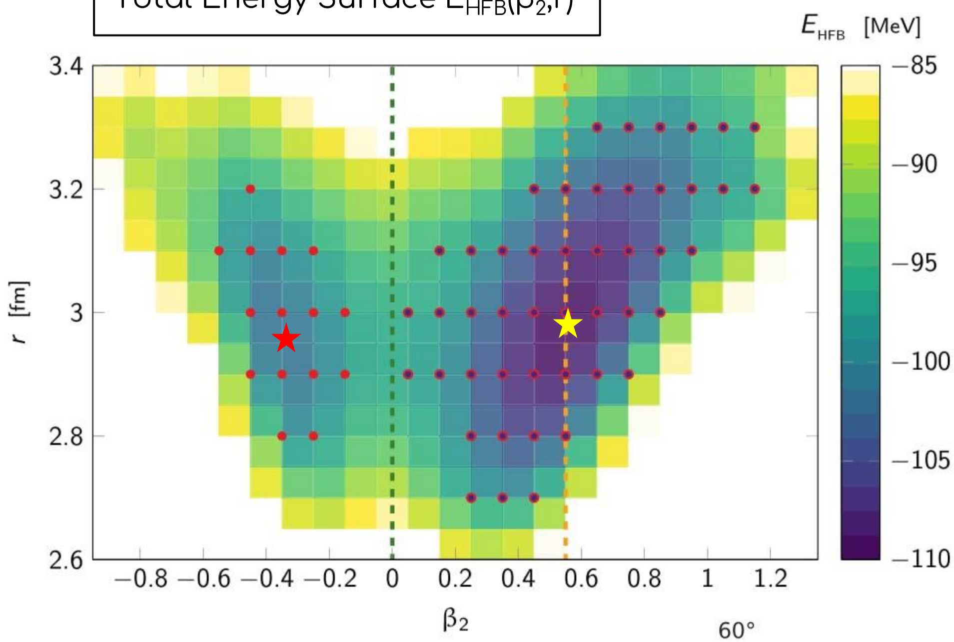

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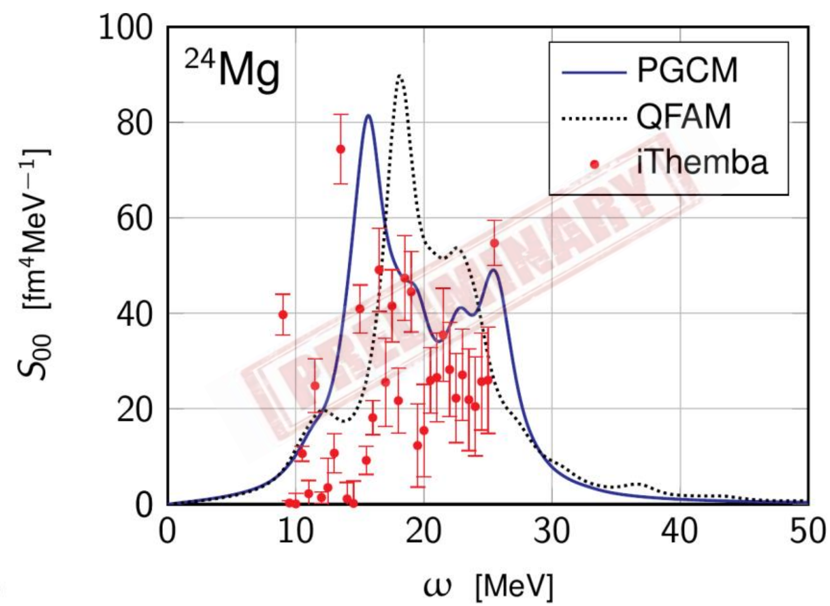
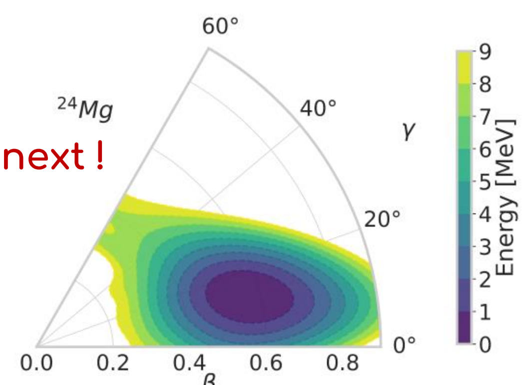


iThemba, Bahini 2021

Triaxiality to be studied next !



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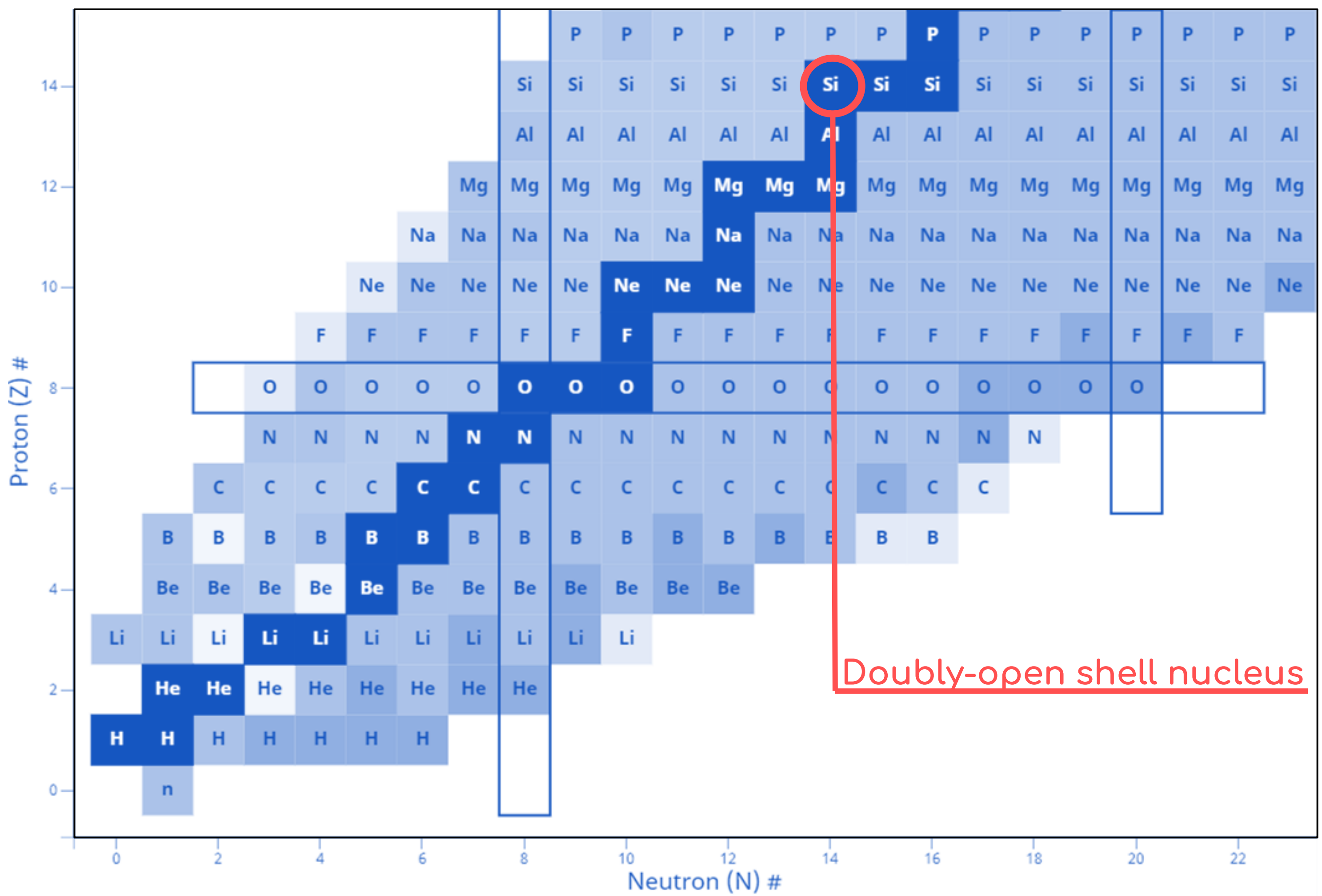
Deformation effects in ^{28}Si



Deformation effects in ^{28}Si

Difficulty

(1) [Jenkins et al., 2012]

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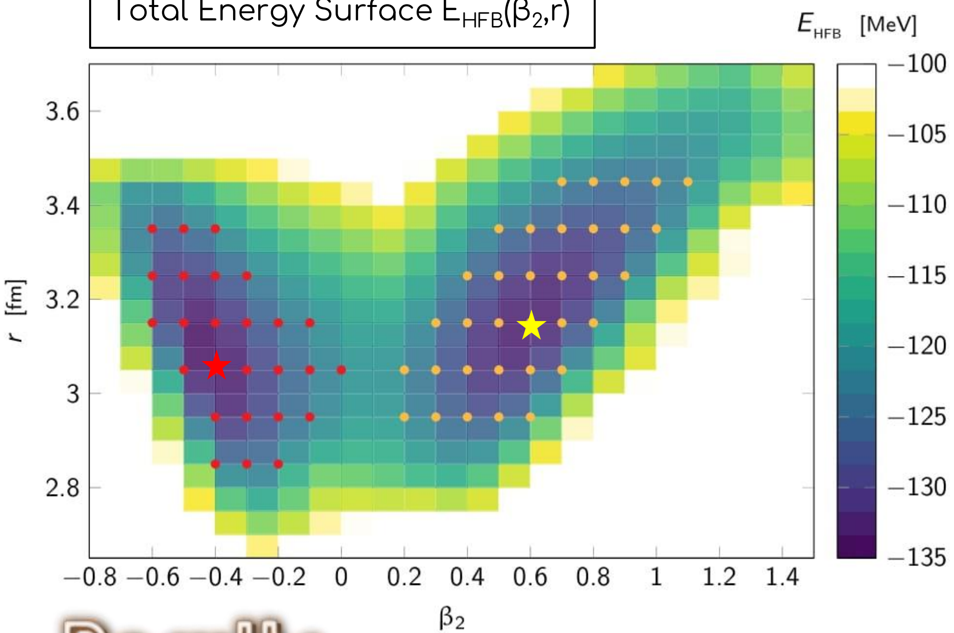

Results

Deformation effects in ^{28}Si

Difficulty

Deformation

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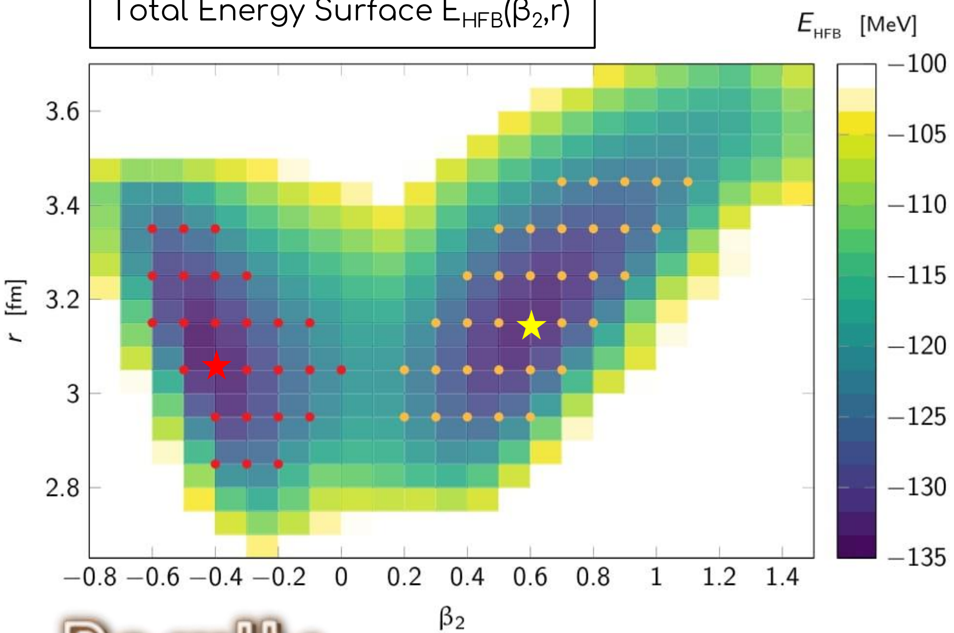

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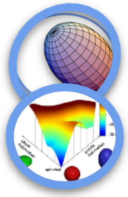

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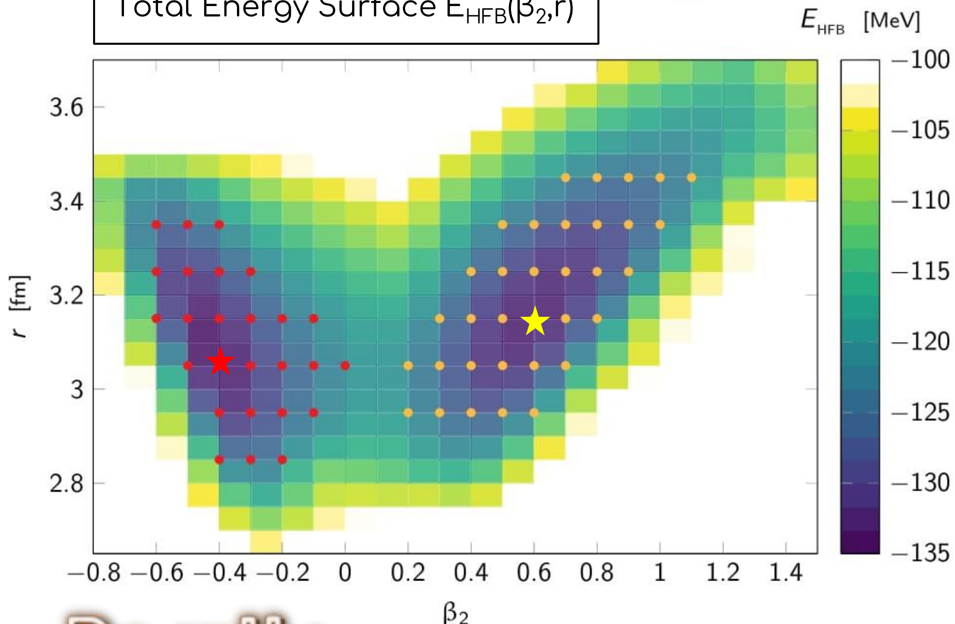

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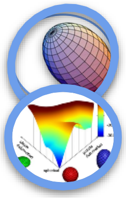

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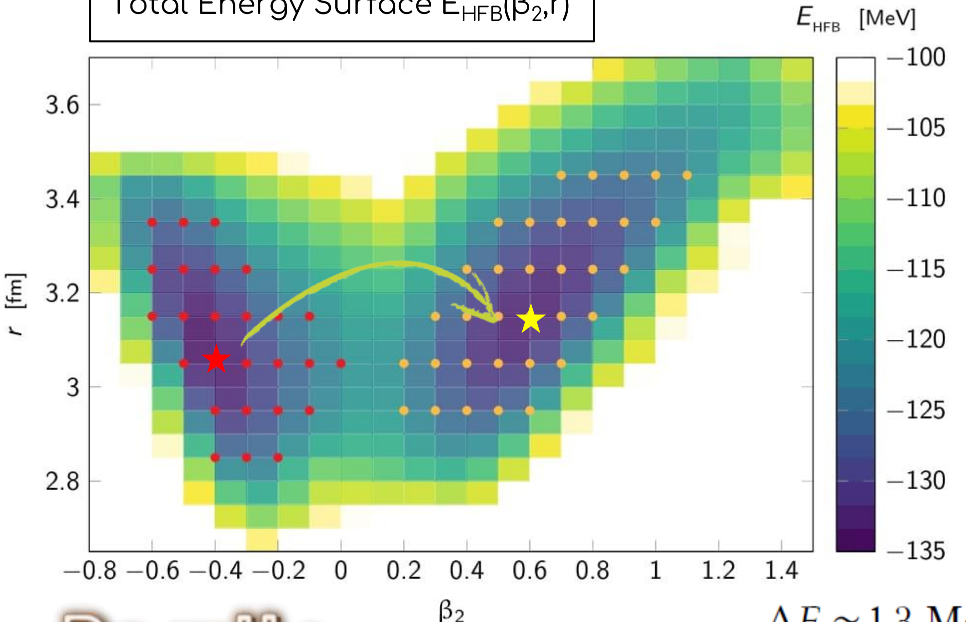


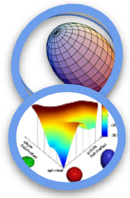
$\Delta E \approx 1.3$ MeV

Results

- Oblate minimum and prolate shape isomer

Deformation effects in ^{28}Si

Difficulty



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Shape coexistence ? (1)

(1) [Jenkins et al., 2012]

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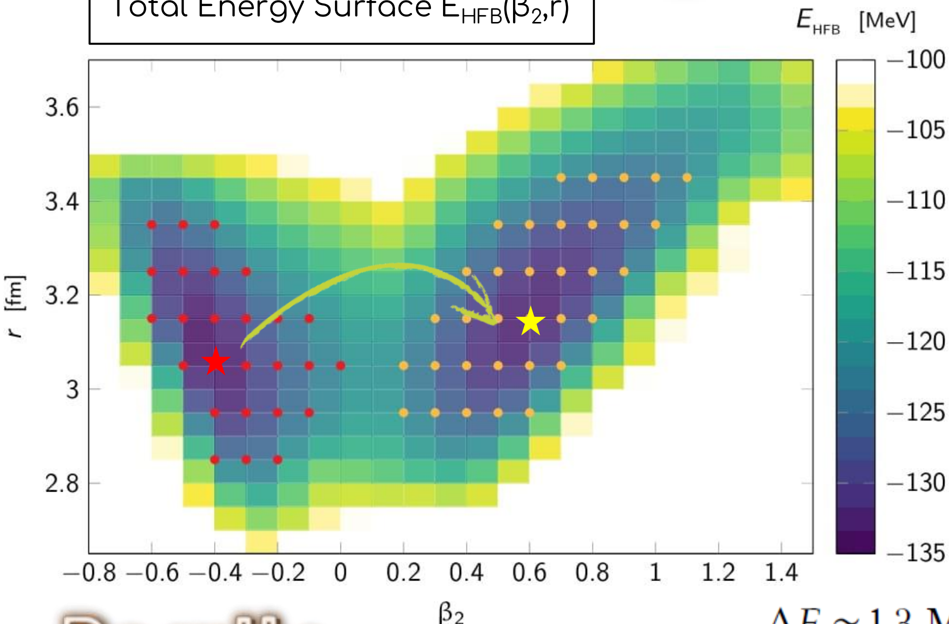

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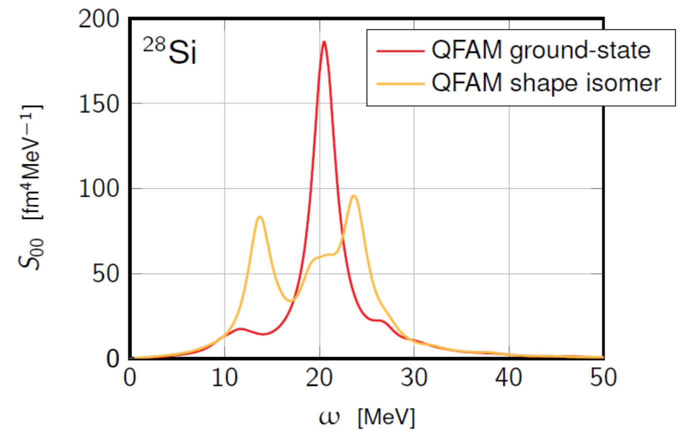
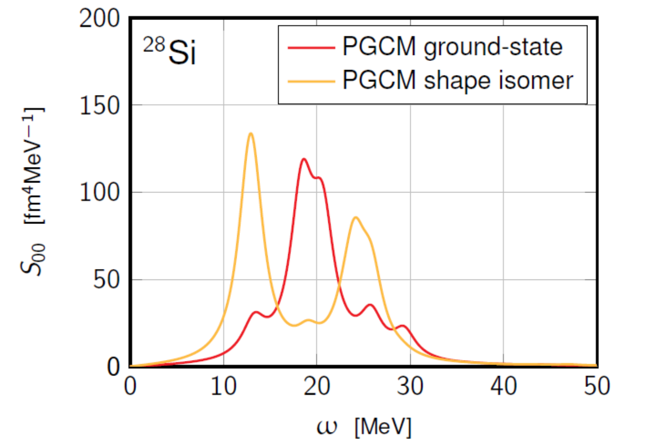
Monopole Strength





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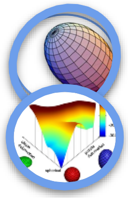

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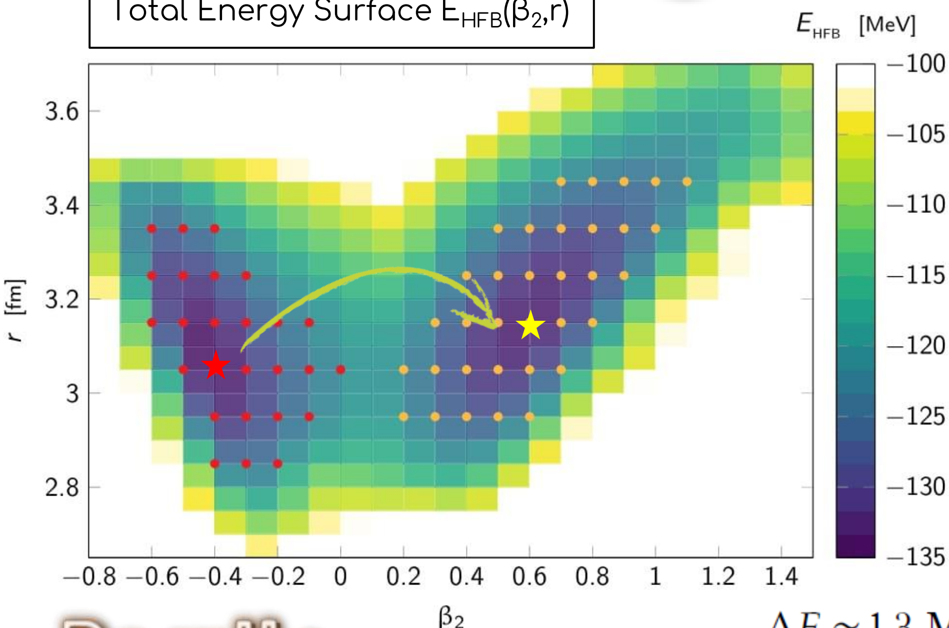

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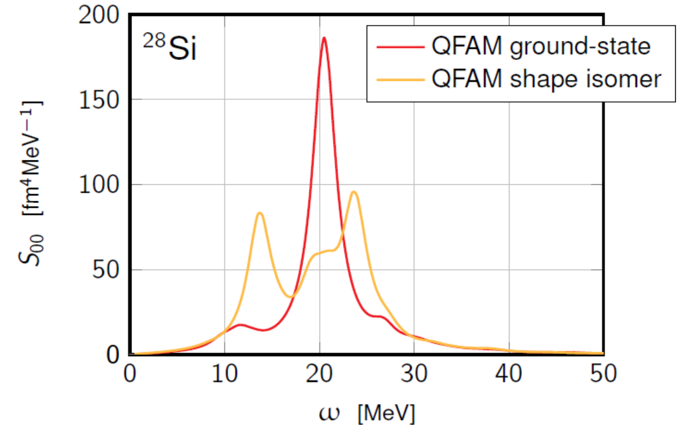

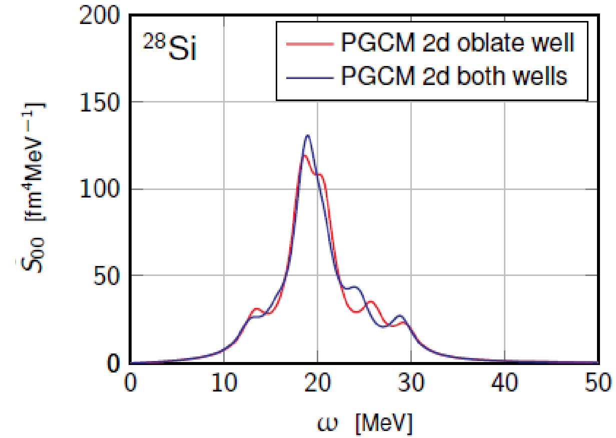

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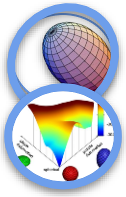

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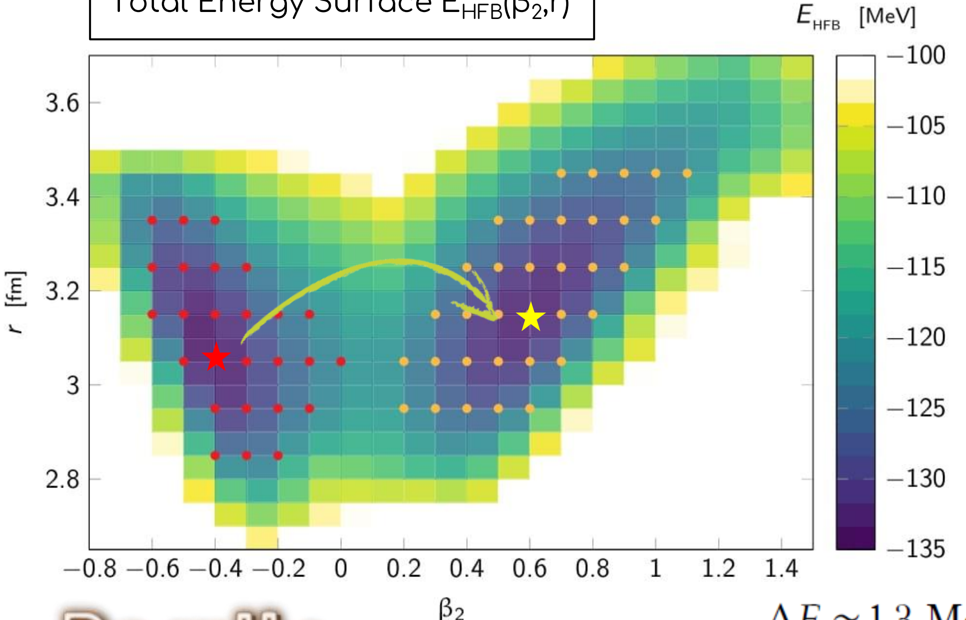

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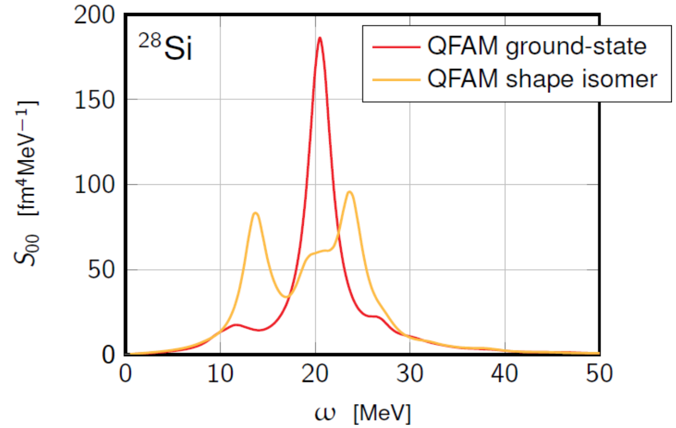

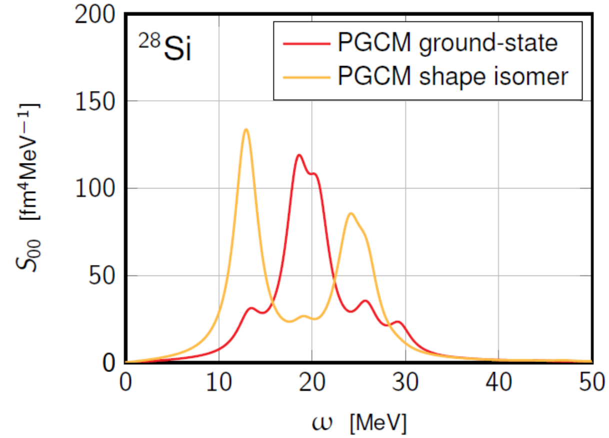

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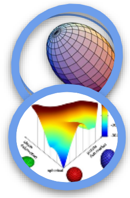

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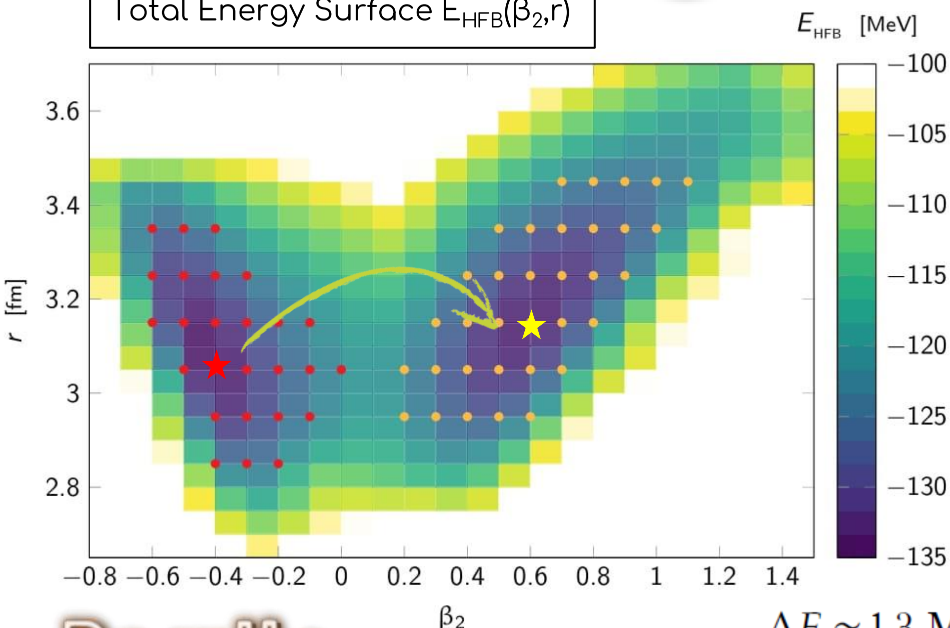

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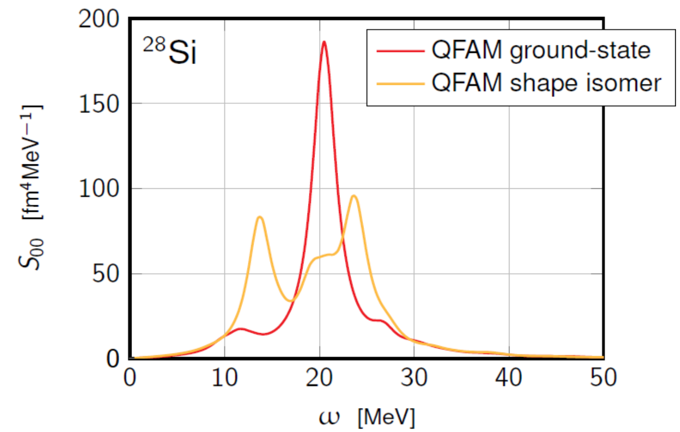

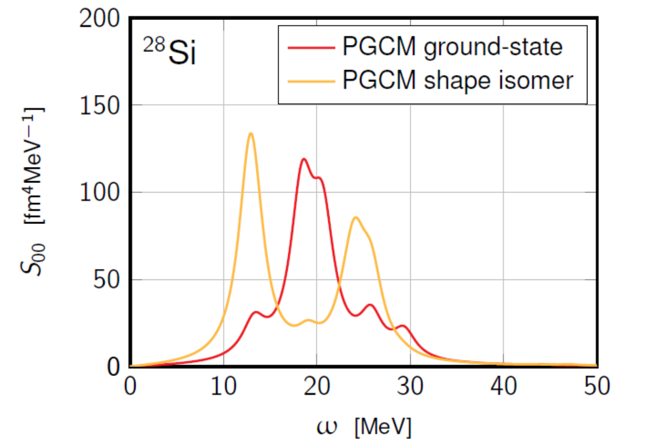

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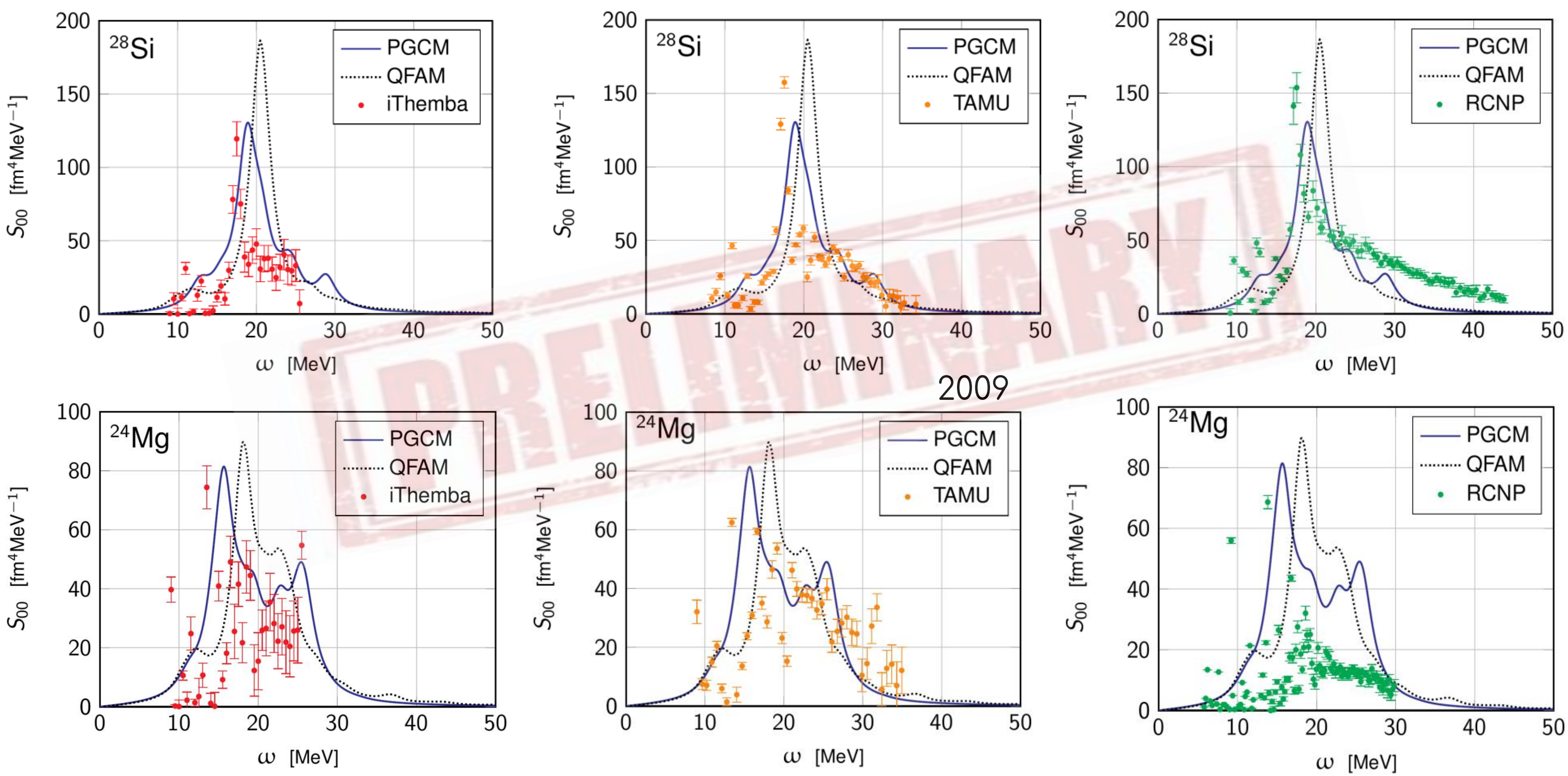
Experimentally accessible ?

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

Plan of the complete study

- [x] Static quadrupolar deformation
- [x] Coupling to quadrupolar vibrations
- [x] Shape isomers
- [ ] Theoretical comparison of moment computation
- [ ] Hamiltonian uncertainty through different chiral EFT orders
- [ ] Pairing: isospin dependence and coupling to pairing vibration
- [ ] Bubble structure (^{34}Si and ^{36}S)
- [ ] Nuclei of current experimental interest (^{68}Ni and ^{70}Ni) [ACTAR TPC]

Thanks for the attention

CEA DRF

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CEA DES

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CEA DAM

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Antoine Roux

INFN

Gianluca Colò
Danilo Gambacurta

Technische Universität Darmstadt

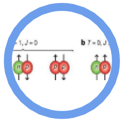
Alexander Tichai

KU Leuven

Pepijn Demol

Pairing effects in ^{20}O

Difficulty



Superfluidity

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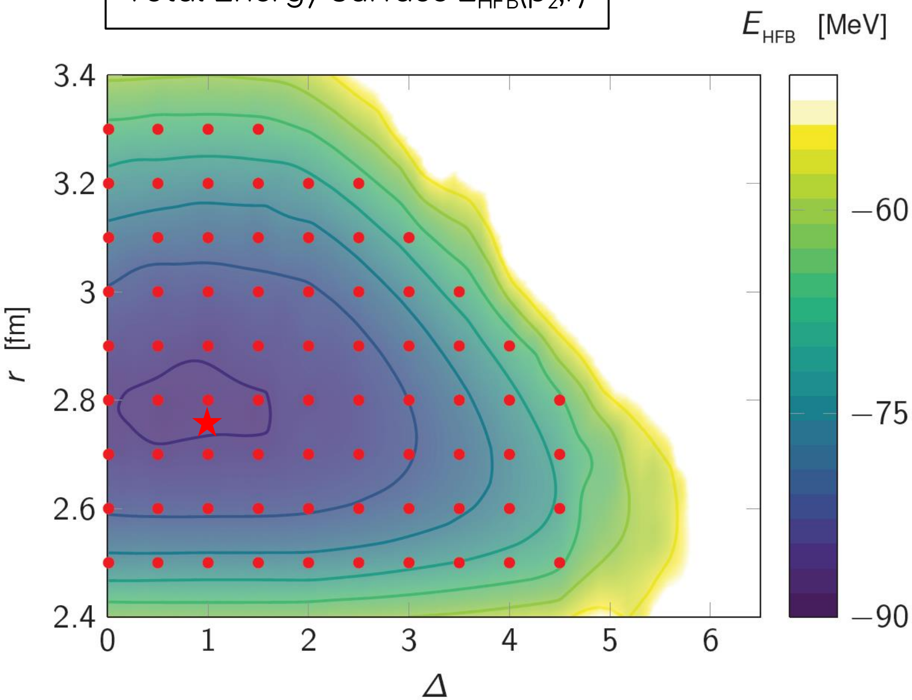

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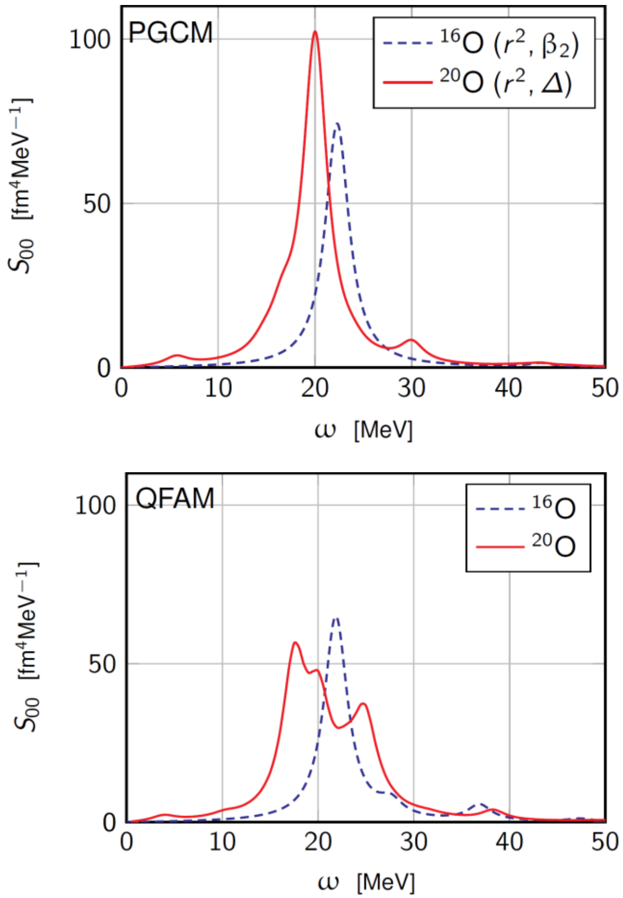

In QRPA another mode seems to be important !