

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

Methods, uses and recent results

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SUPERVISORS

Thomas Duguet Vittorio Somà

July 21st, 2023

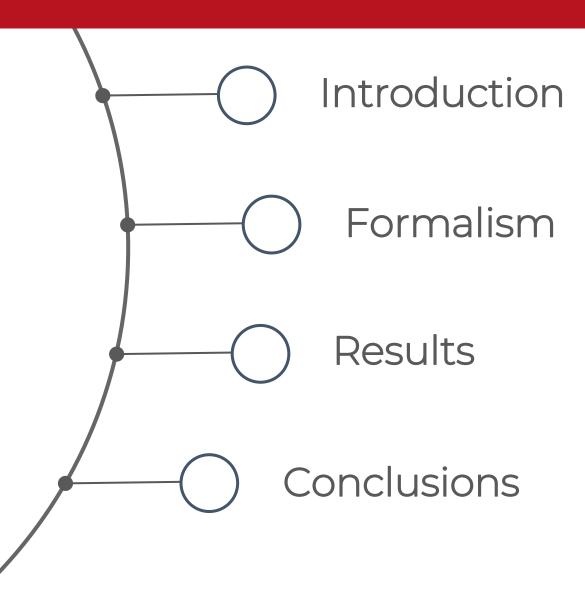
XVII International Symposium on Capture Gamma-Ray Spectroscopy and Related Topics – CGS17

ILL Grenoble

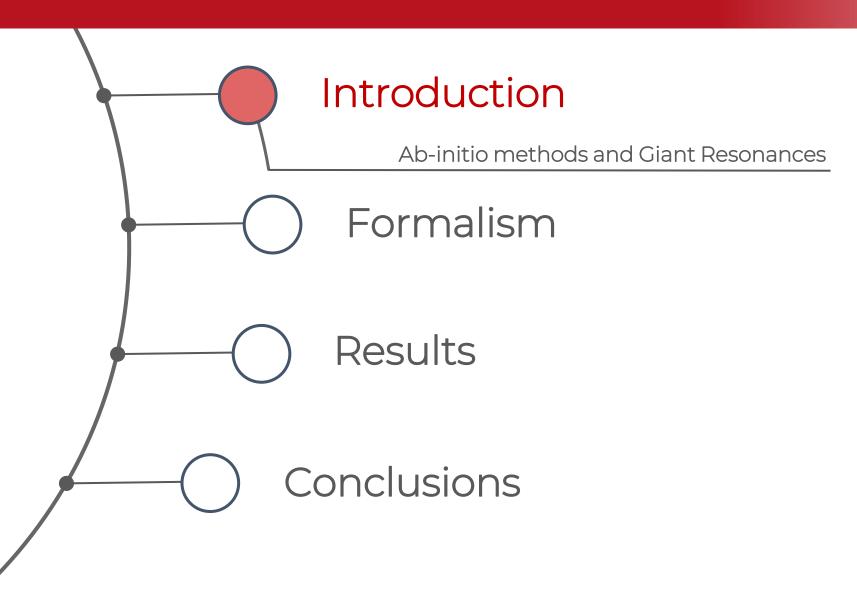




Outline



Outline



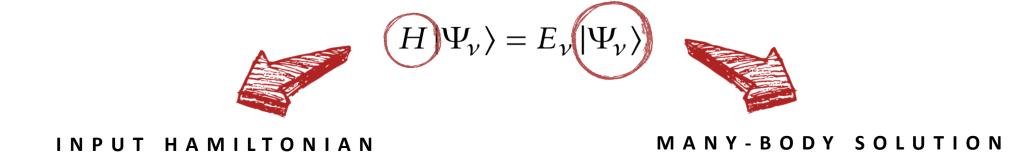
Global philosophy

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

Global philosophy



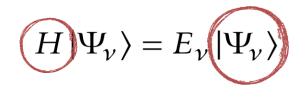
Global philosophy



Global philosophy

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





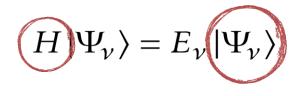


INPUT HAMILTONIAN

Global philosophy

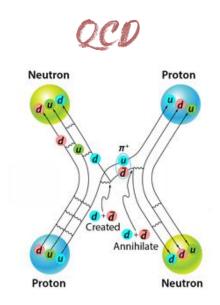
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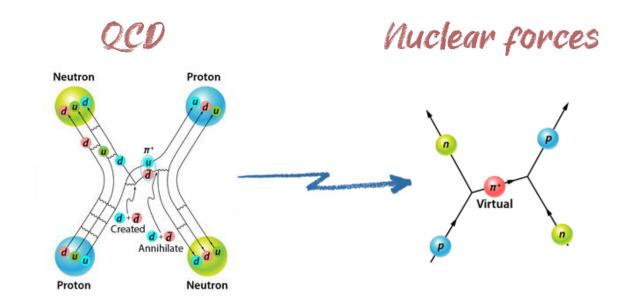
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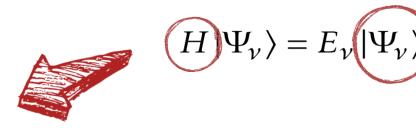






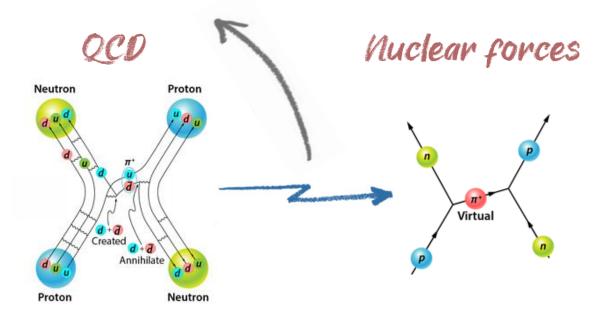
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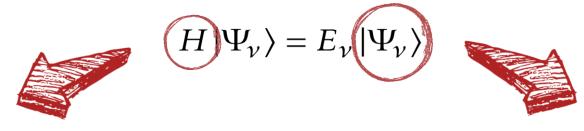


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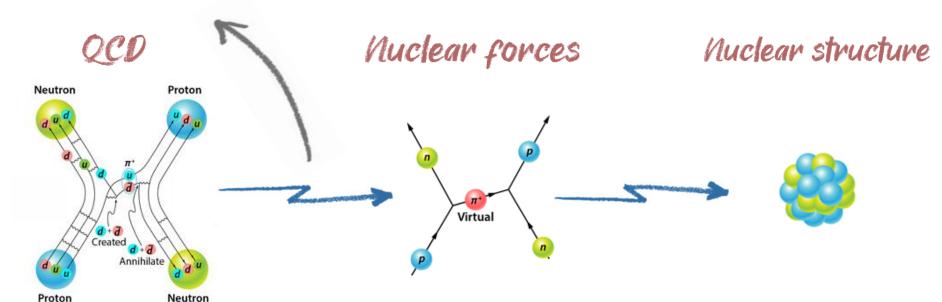


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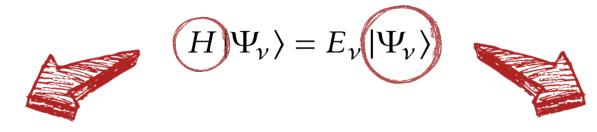


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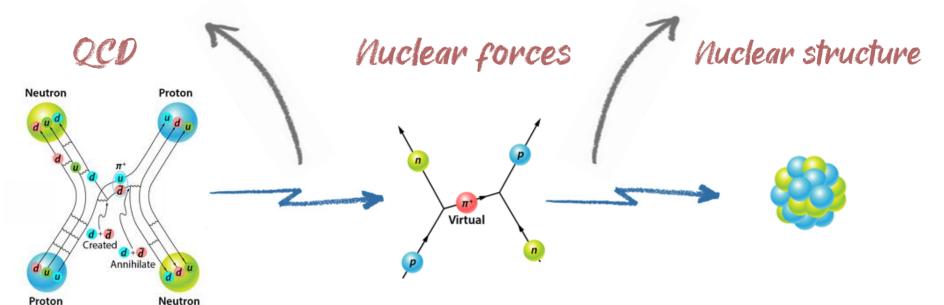


Global philosophy

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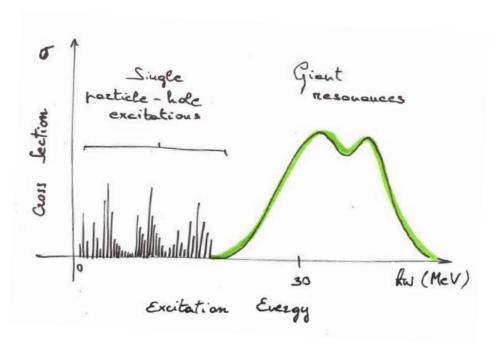


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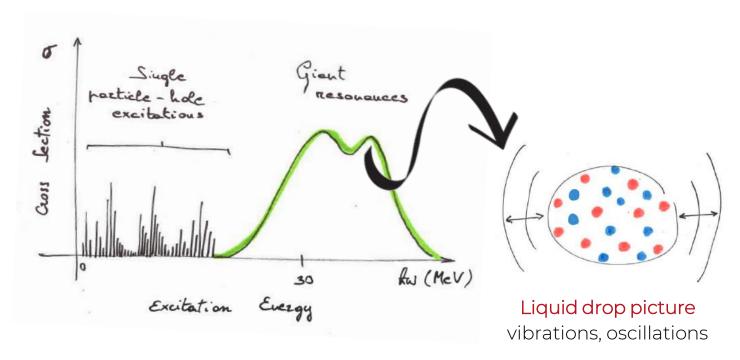
Dual nature of nucleus

- single-particle features
- collective behaviour



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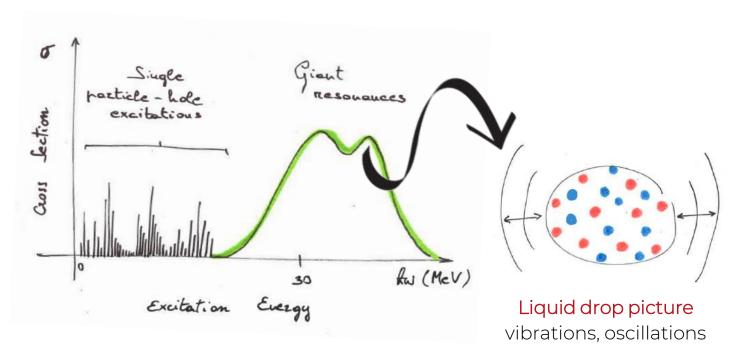


Giant Resonances (GRs)

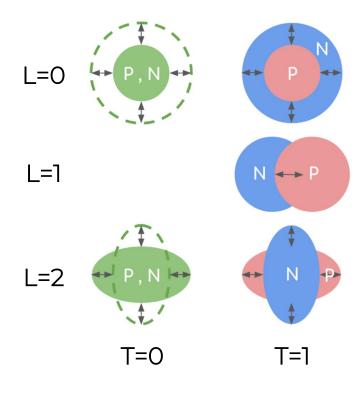
clearest manifestation of collective motion

Dual nature of nucleus

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Giant Resonances (GRs)



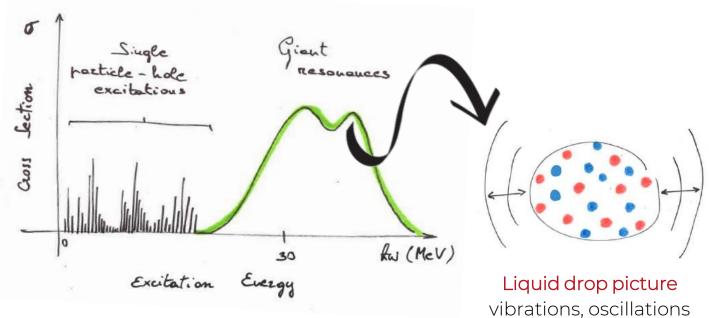
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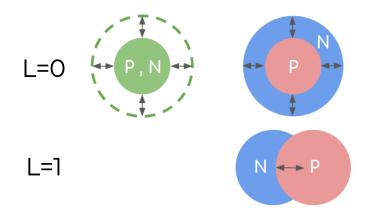
Compression-mode resonances

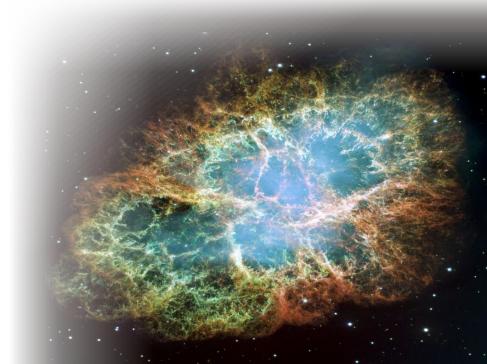
- Incompressibility of nuclear matter K_{∞}
- Nuclear Equation of State
- Core-collapse supernova explosion



Giant Resonances (GRs)

clearest manifestation of collective motion





What is it?

- Collective excitation (breathing mode)
- Involving most if not all the nucleons
- Coherent particle-hole excitations

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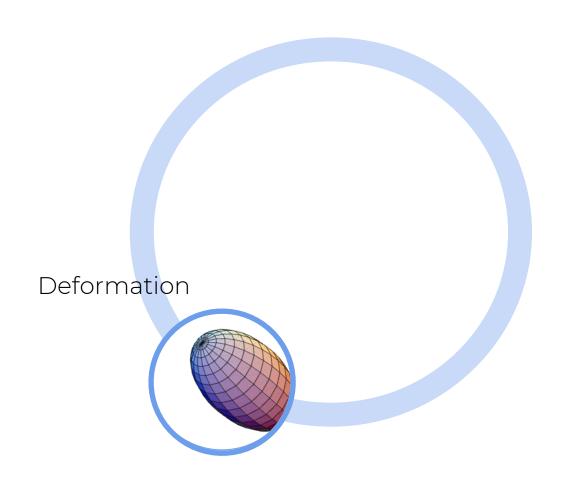
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- Renewed experimental interest
- Investigate new physics

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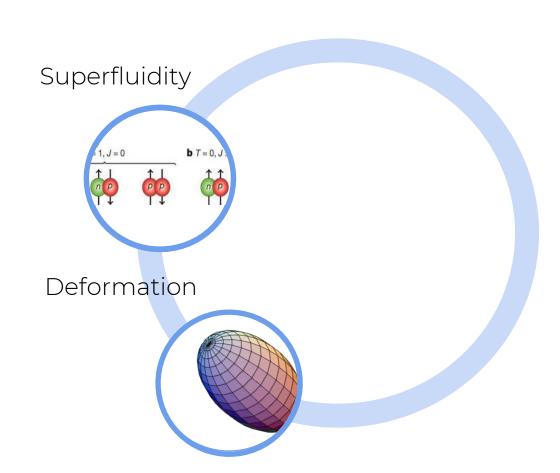
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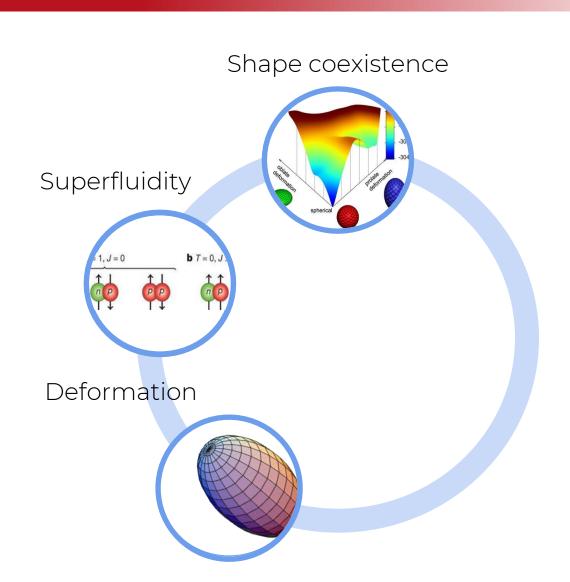
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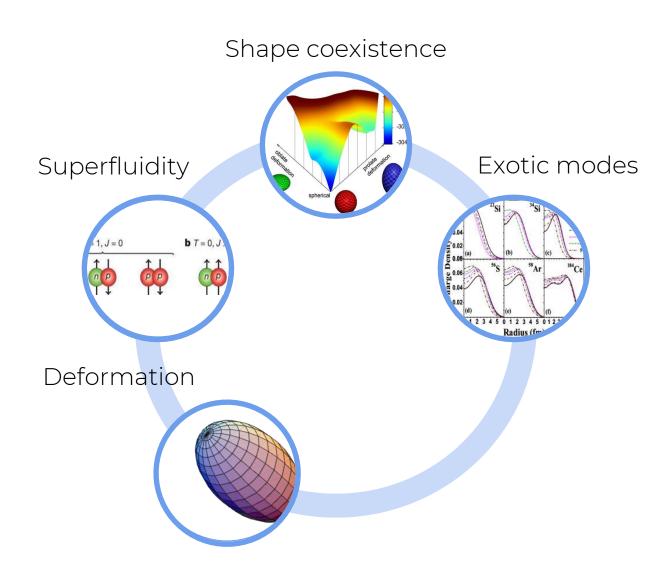
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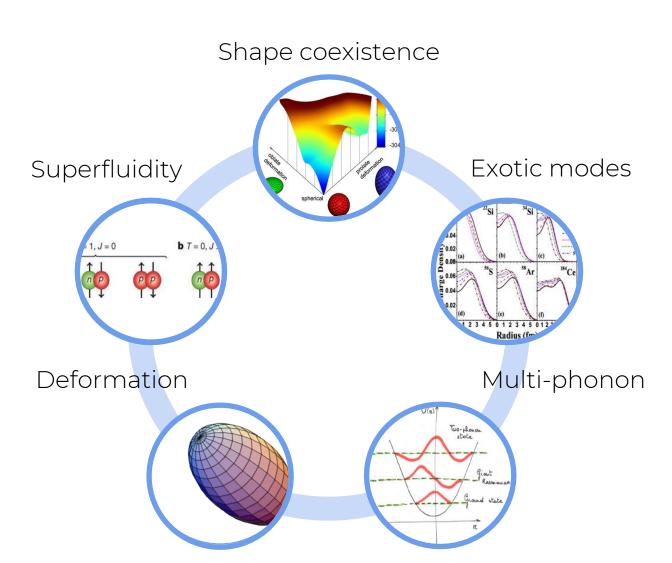
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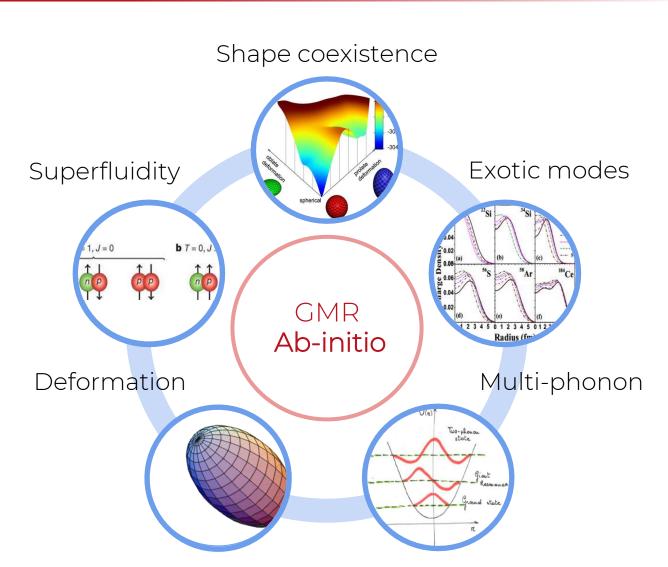
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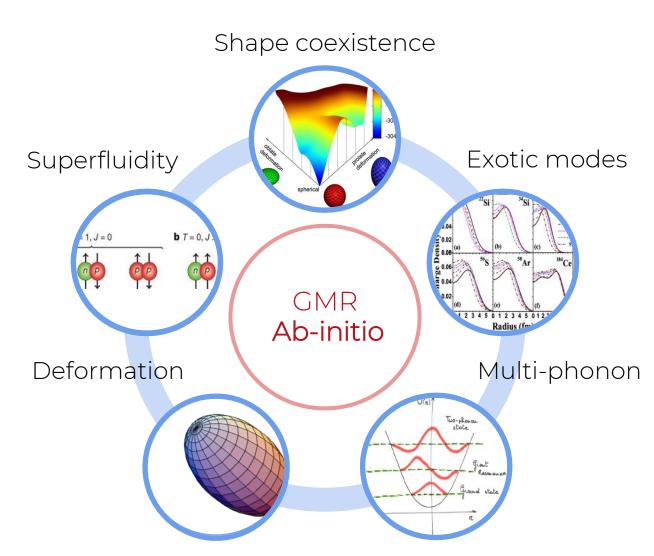
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Why studying again GMR?

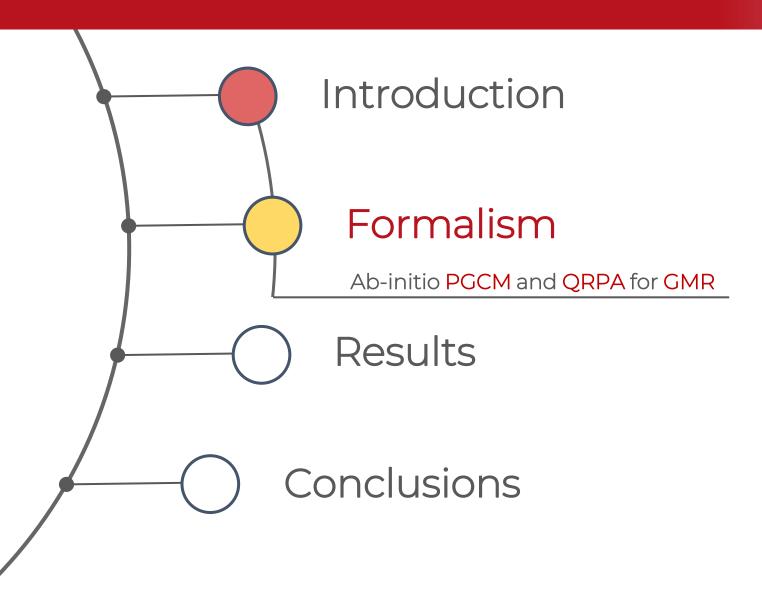
- Renewed experimental interest
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Much is still to be understood!

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

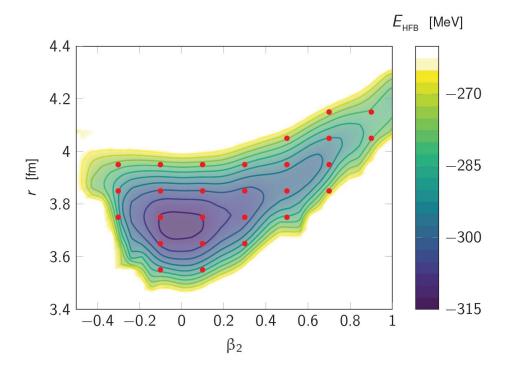


Outline



Schrödinger equation

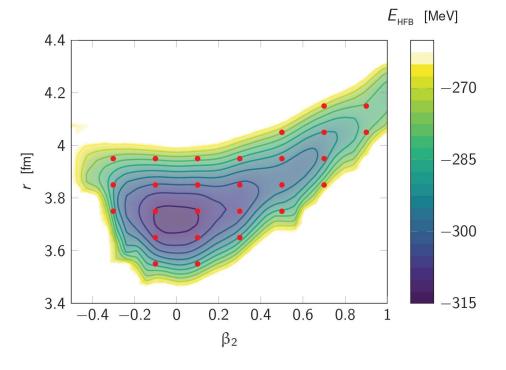
$$H|\Psi_{\nu}\rangle = E_{\nu}|\Psi_{\nu}\rangle$$



Schrödinger equation

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Open-shell systems



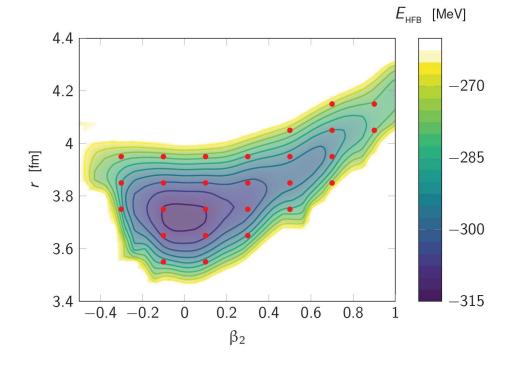
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Open-shell systems



Strong static correlations



Schrödinger equation

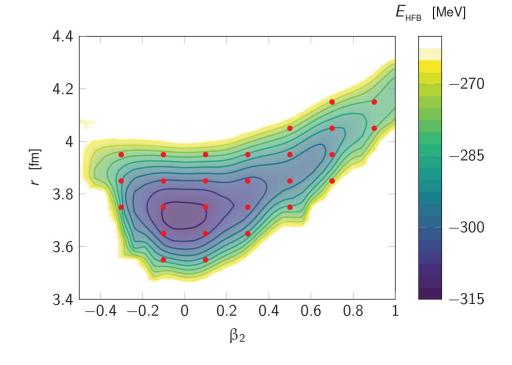
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Open-shell systems

Symmetry-breaking reference states



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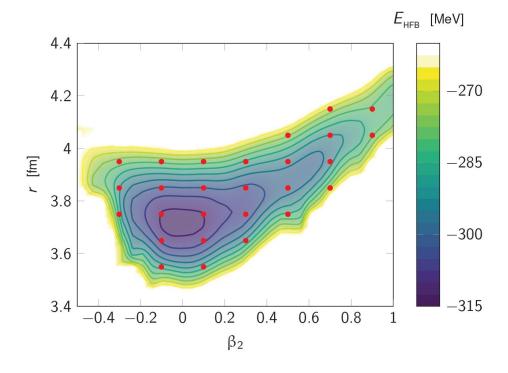
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Strong static correlations

1 Constrained HFB solutions

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



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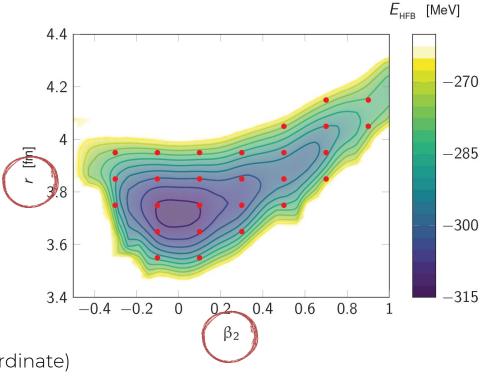
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Strong static correlations

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 3.4 Generator coordinates (can be in principle whatever coordinate)



Schrödinger equation

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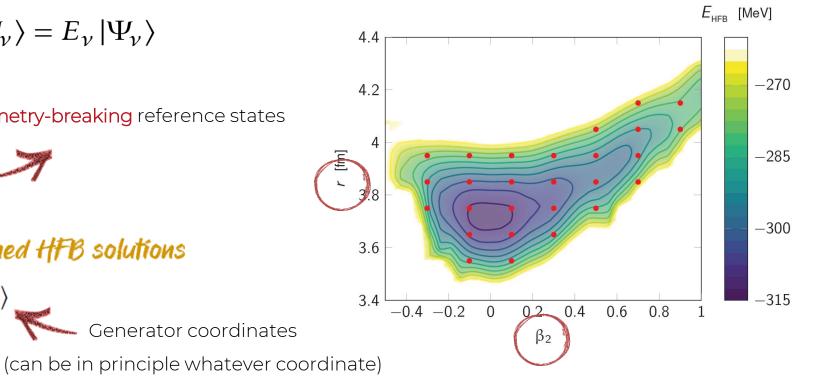
Strong static correlations

Constrained HFB solutions

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

PGCM Ansatz

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



Schrödinger equation

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Open-shell systems

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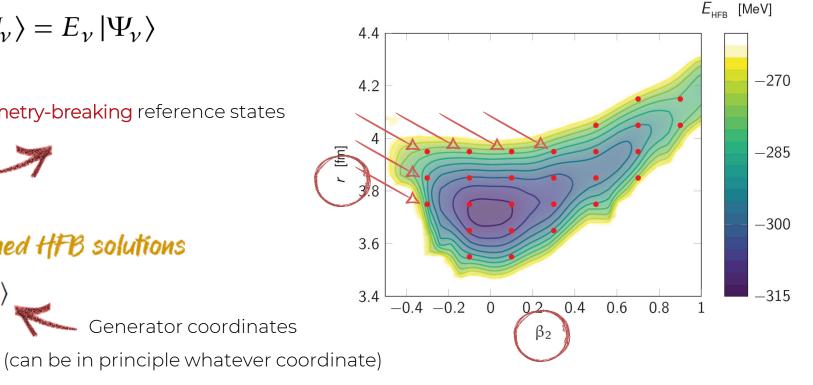
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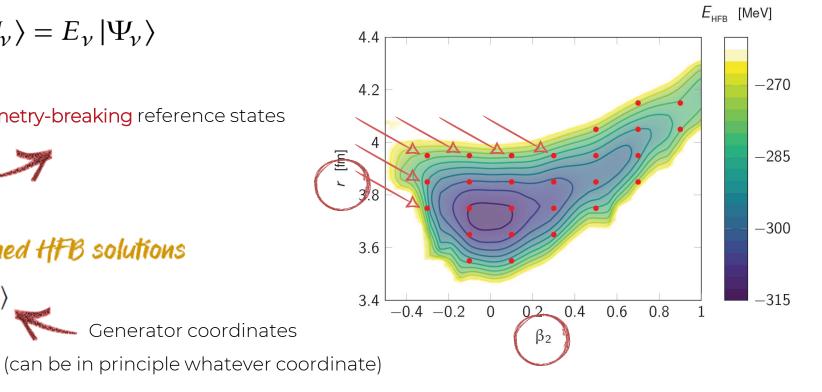
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PGCM Ansatz

Linear coefficients



Projected Generator Coordinate Method

Schrödinger equation

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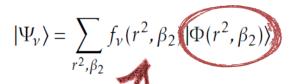
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Generator coordinates

(can be in principle whatever coordinate)



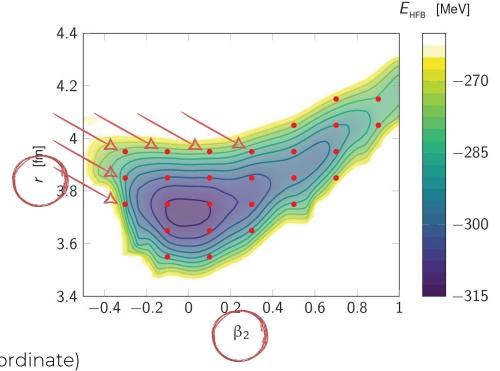


Linear coefficients

3 HWG Equation

Variational method

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



Projected Generator Coordinate Method

Schrödinger equation

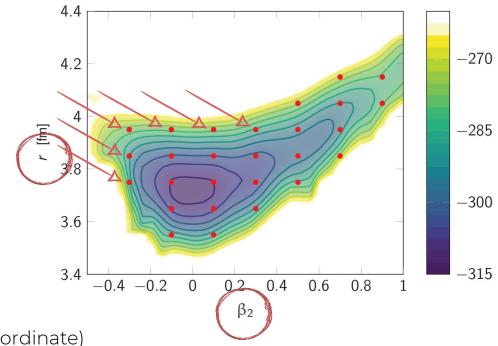
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Schrödinger-like equation

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

Kernels evaluation

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

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

 E_{HFB} [MeV]

Projected Generator Coordinate Method

Schrödinger equation

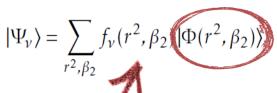
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Diagonalization in a physically-informed reduced Hilbert space

Constrained HFB solutions

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

PGCM Ansatz



Linear coefficients



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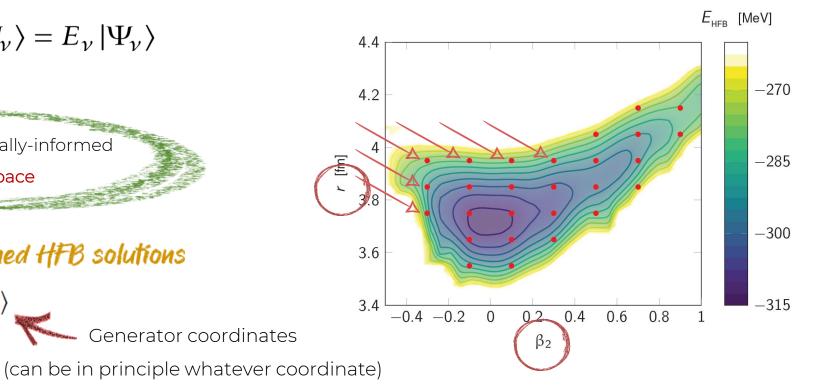
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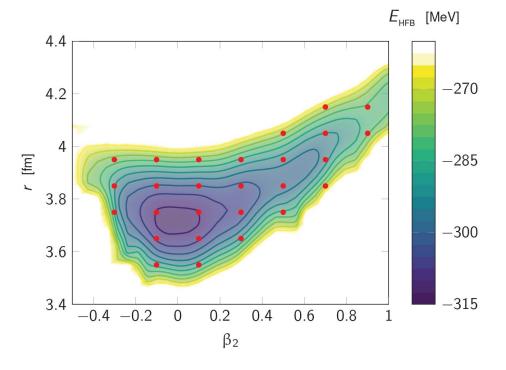
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Thouless theorem

(q can be whatever coordinate)

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

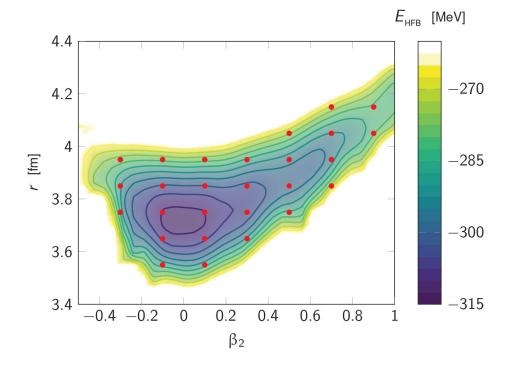


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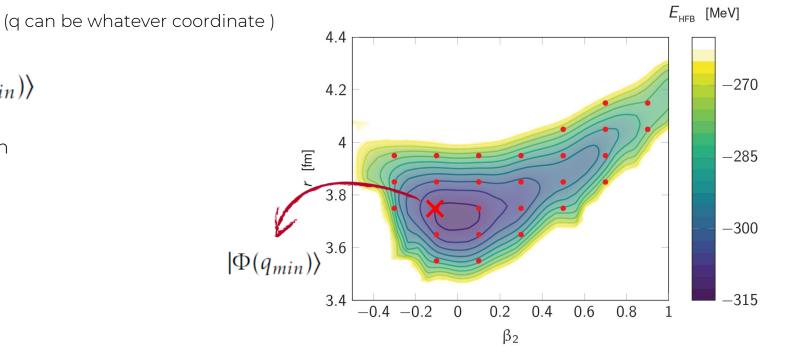
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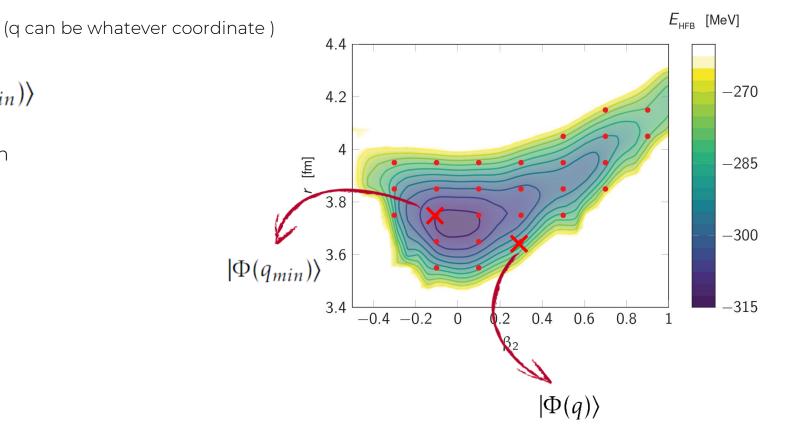
Non-unitary transformation



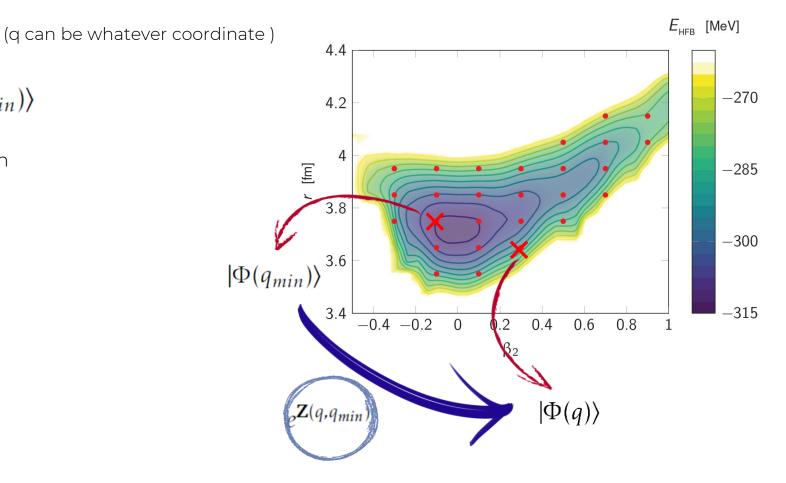
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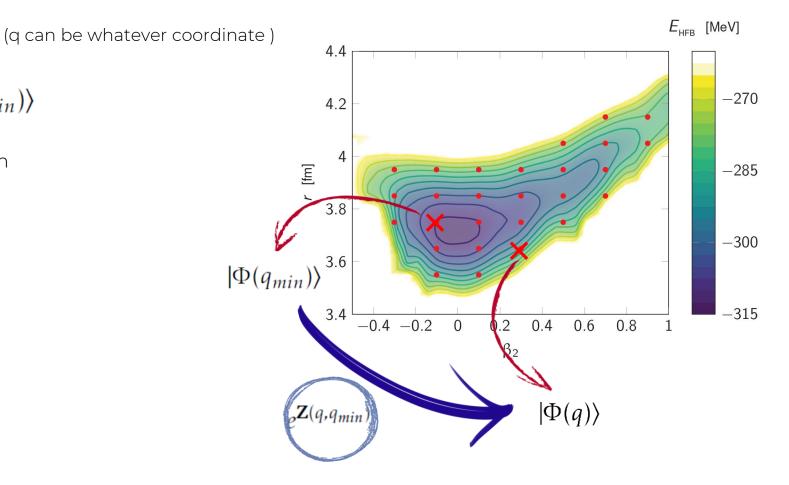
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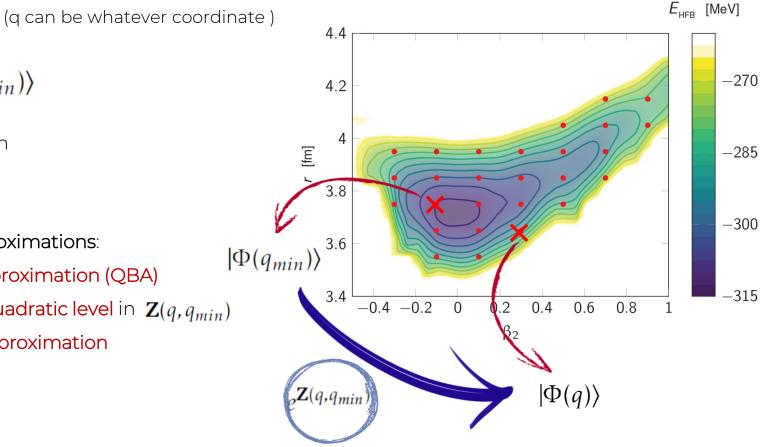
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Solve with two approximations:

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



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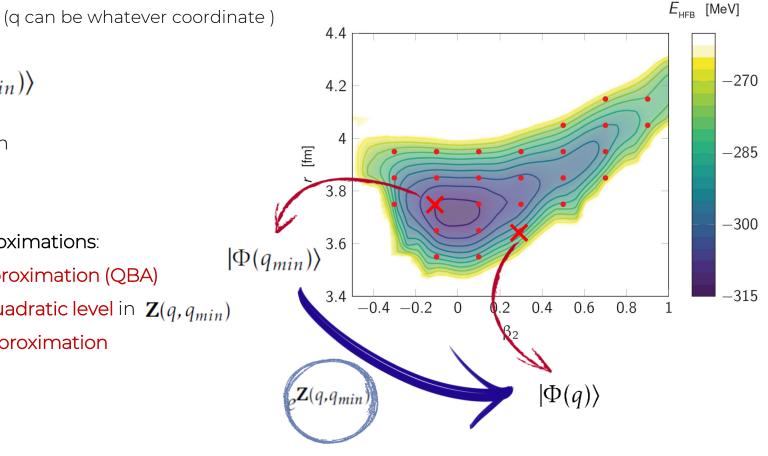
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No coordinates dependency!

All coordinates are explored (differently from PGCM)



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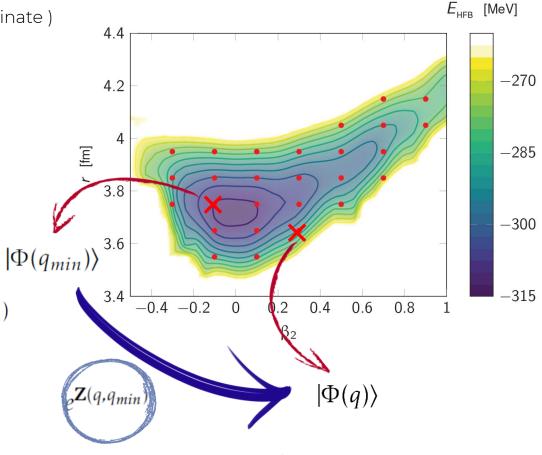
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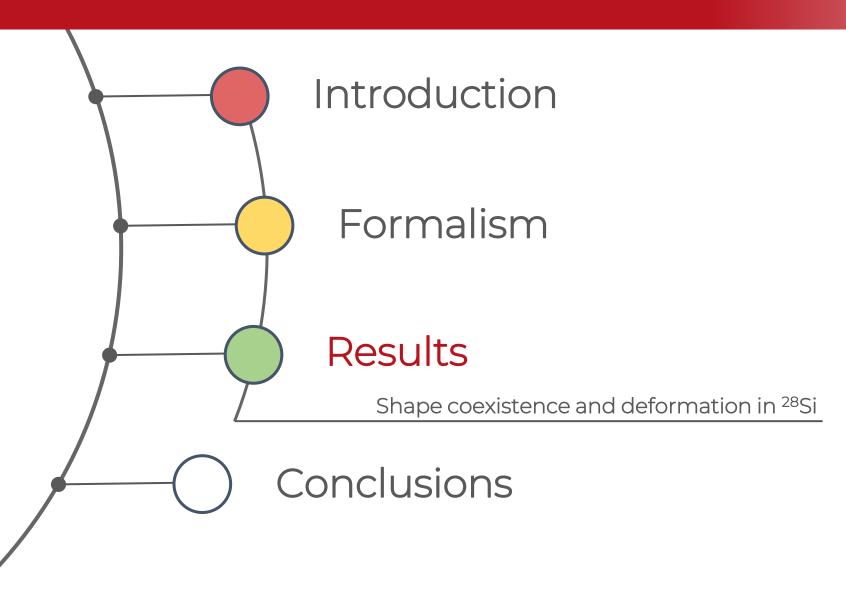


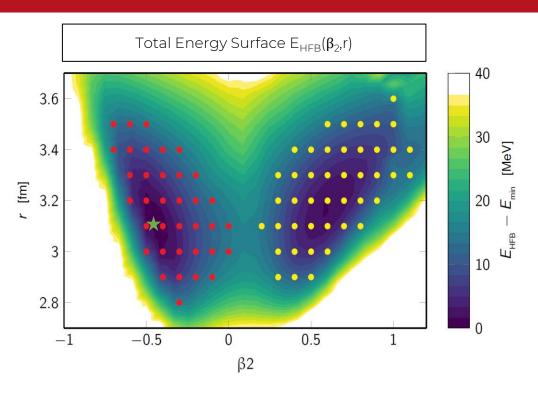


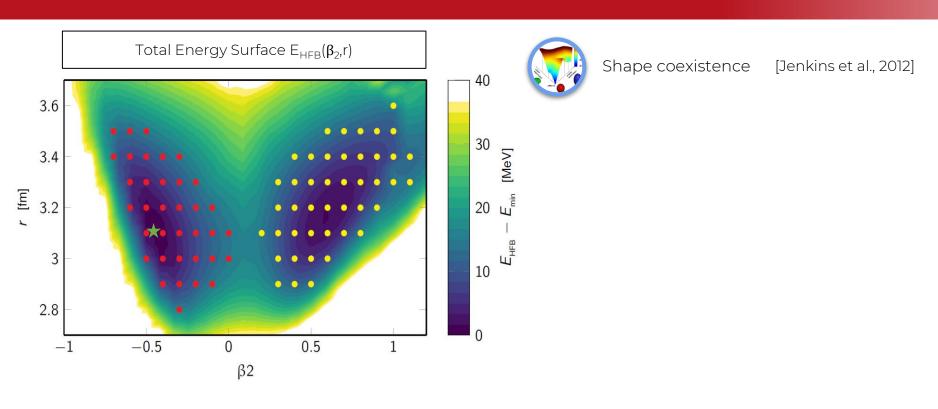
Eventually rewrites as **QRPA**

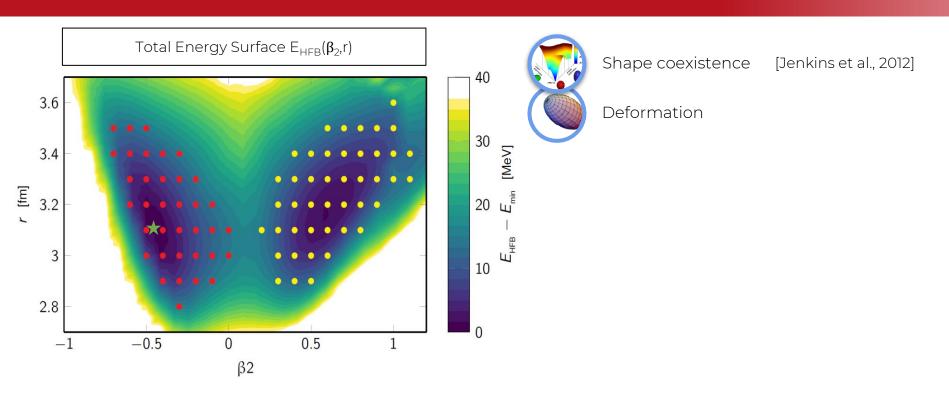
$$\begin{pmatrix} A & B \\ -B^* & -A^* \end{pmatrix}^k \begin{pmatrix} X^{\nu} \\ Y^{\nu} \end{pmatrix} = E^k_{\nu} \begin{pmatrix} X^{\nu} \\ Y^{\nu} \end{pmatrix}$$

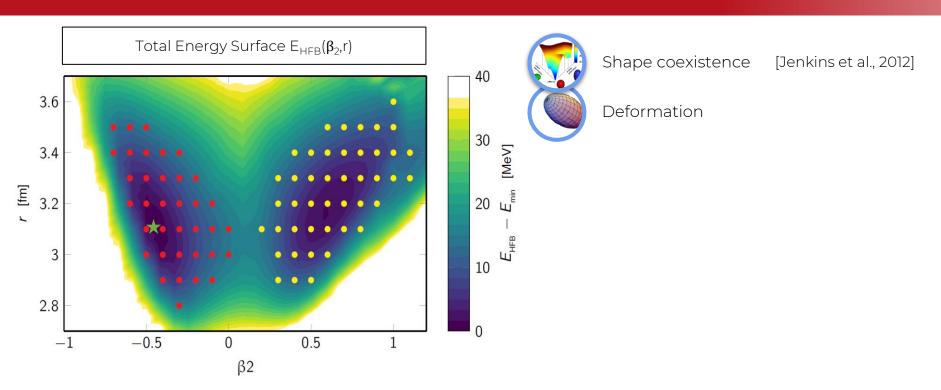
Outline



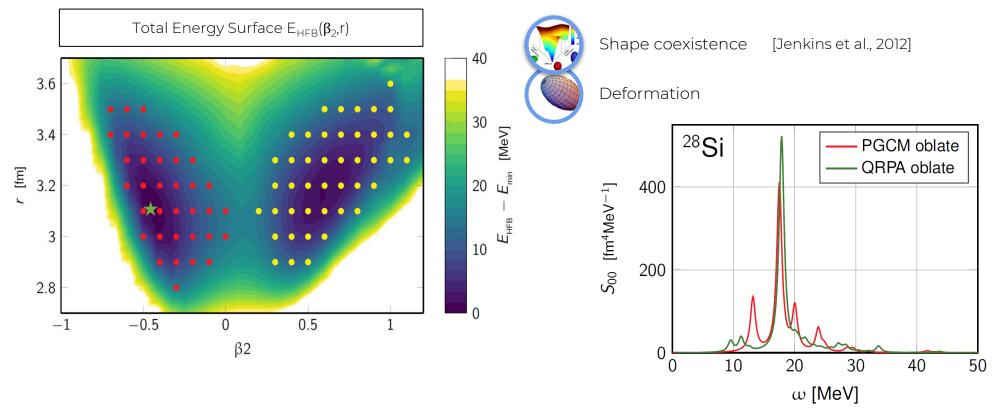




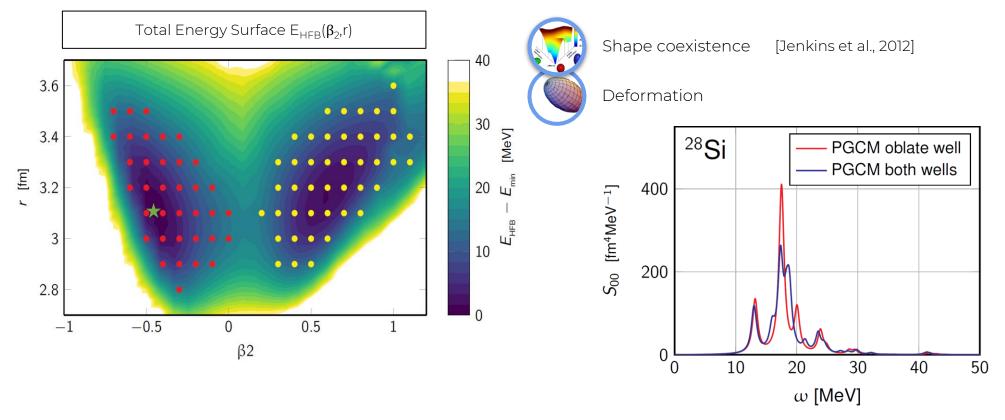




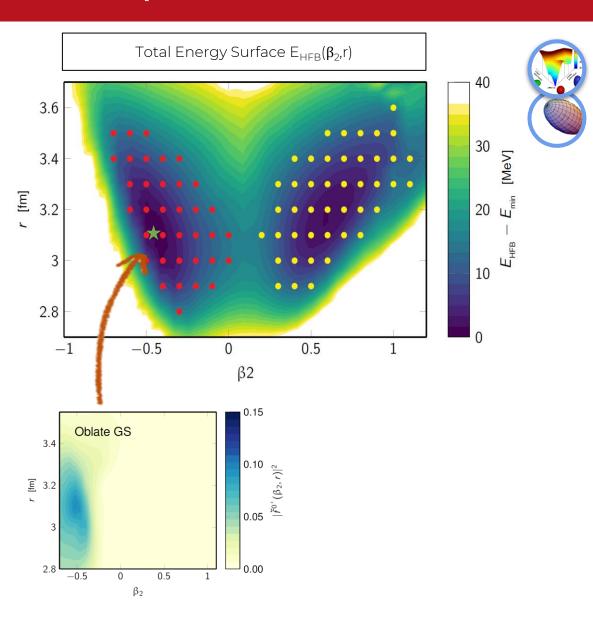
Oblate minimum and prolate-shape isomer



- Oblate minimum and prolate-shape isomer
- Qualitatively similar results QRPA/PGCM
 - QRPA response less fragmented

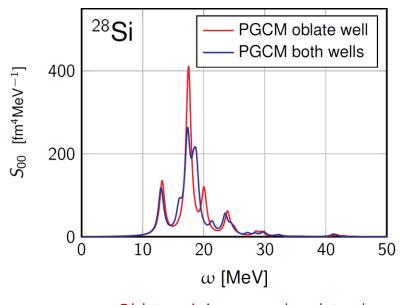


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 - Shape coexistence but no shape mixing

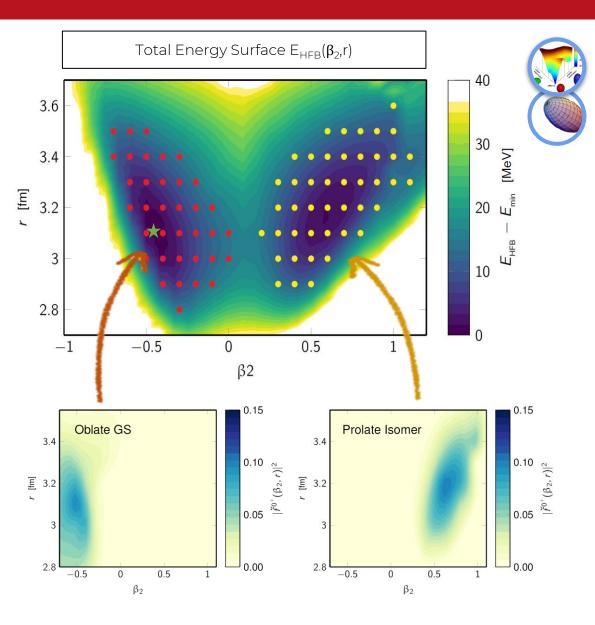


Shape coexistence [Jenkins et al., 2012]

Deformation

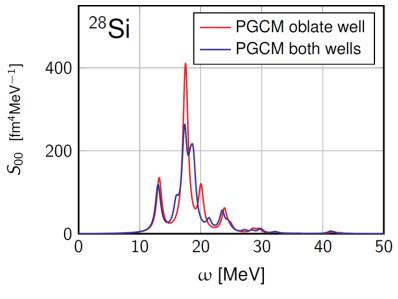


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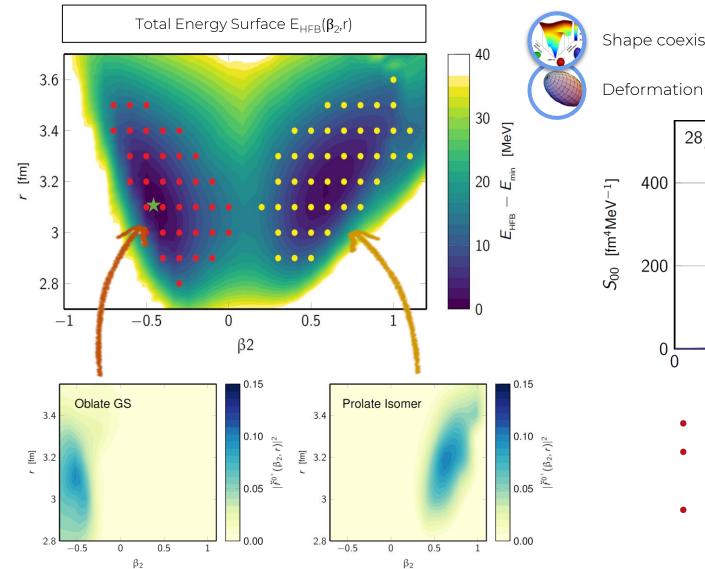
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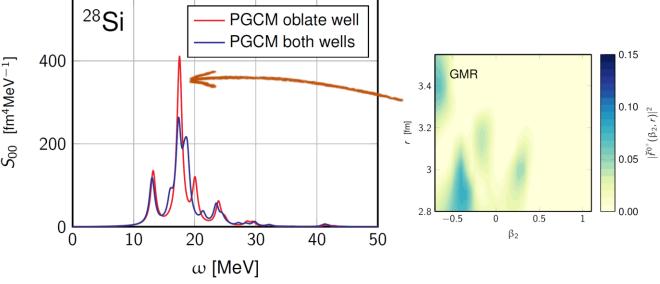


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Shape coexistence effects in 28Si

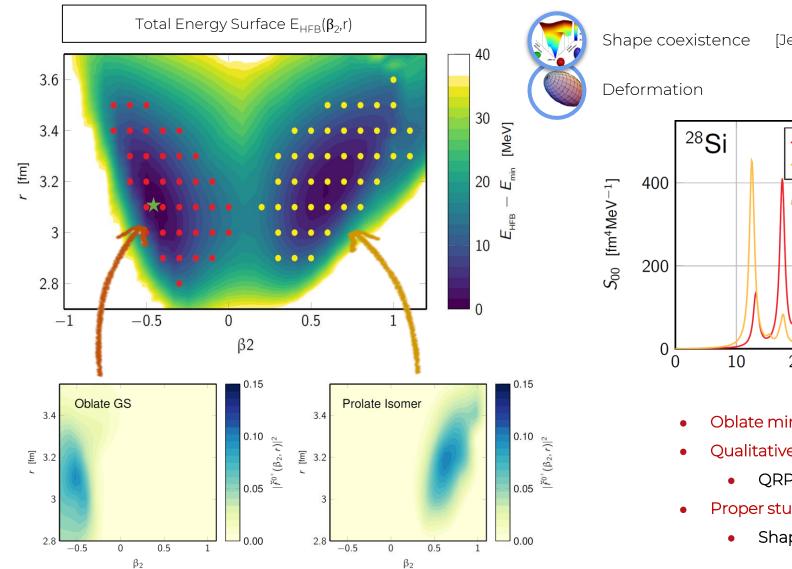


Shape coexistence [Jenkins et al., 2012]

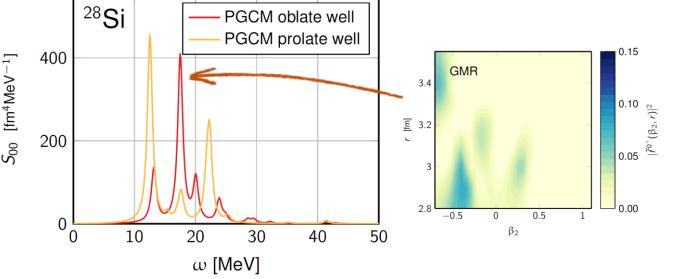


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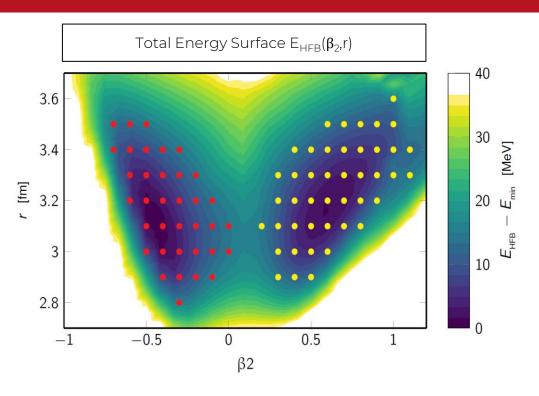
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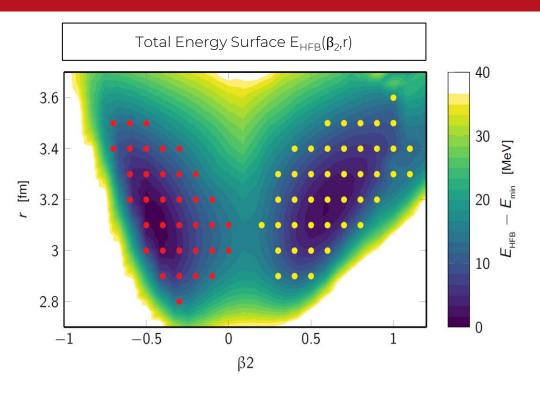


[Jenkins et al., 2012]

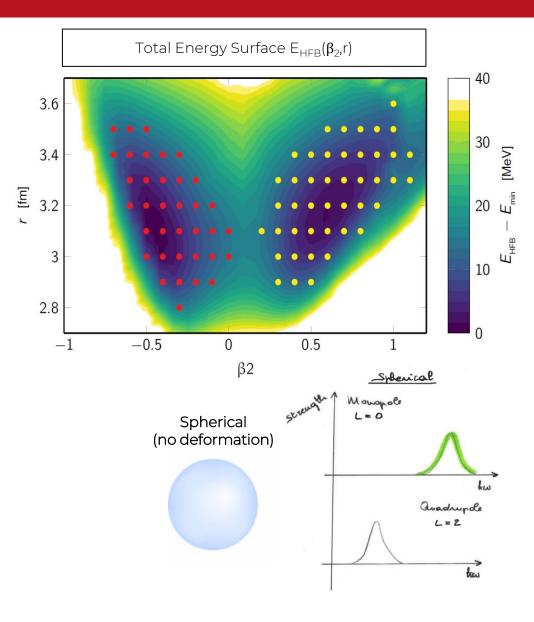


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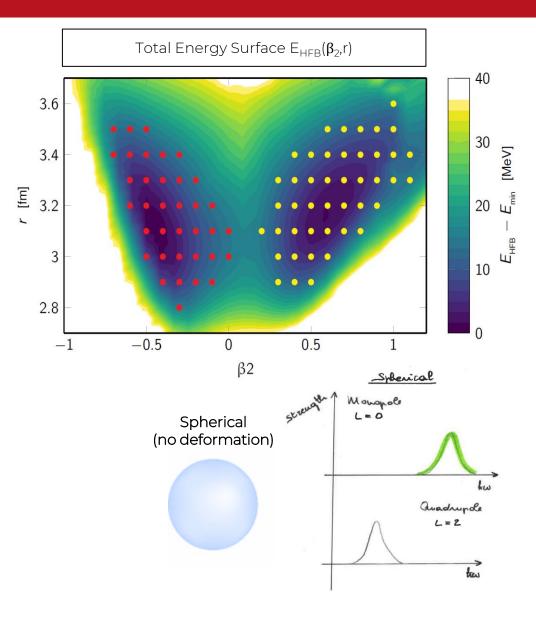




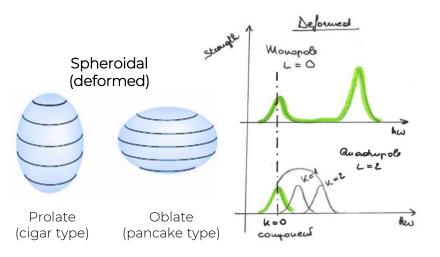
• Focus on the prolate-shape isomer

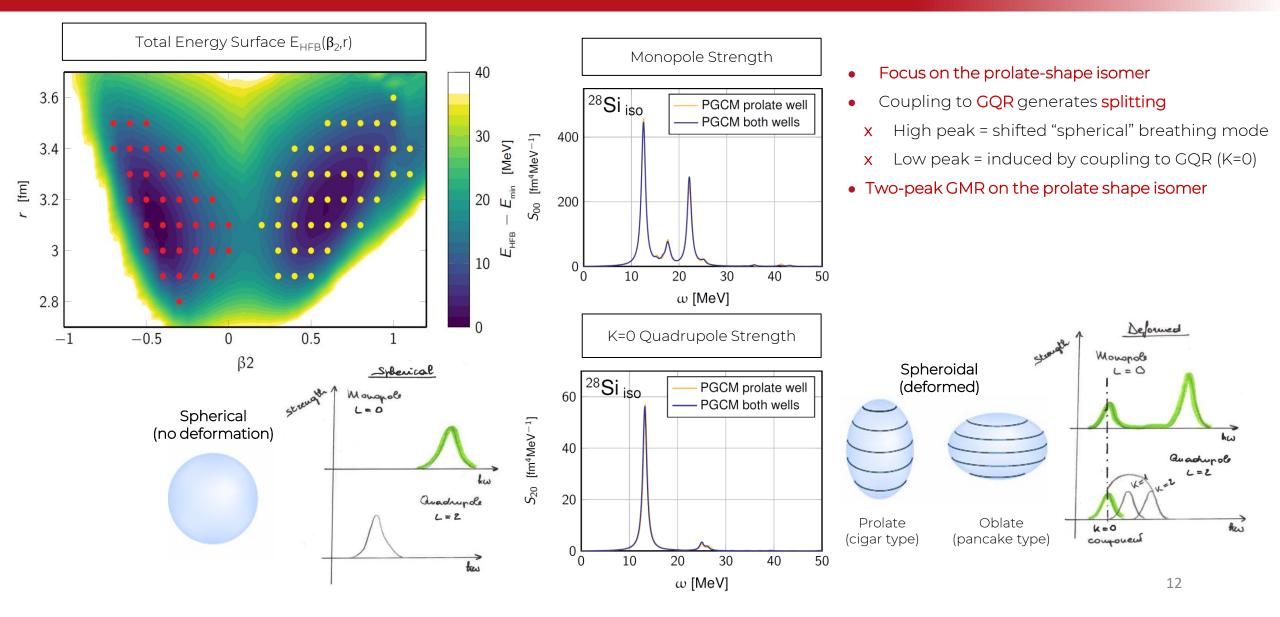


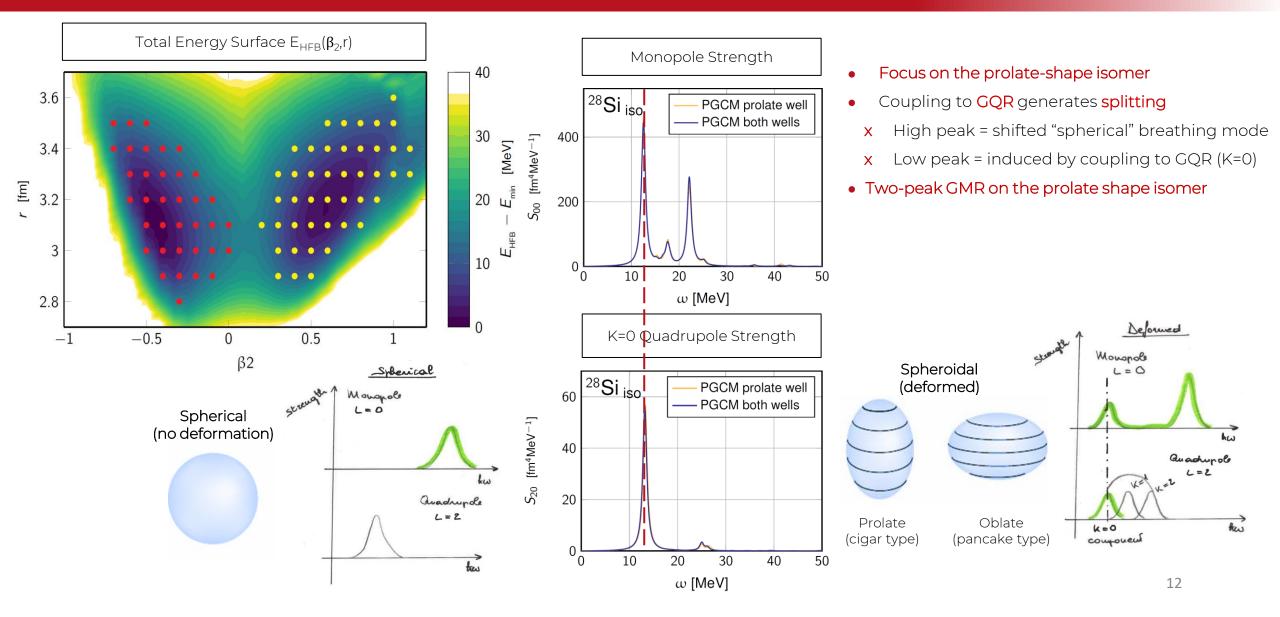
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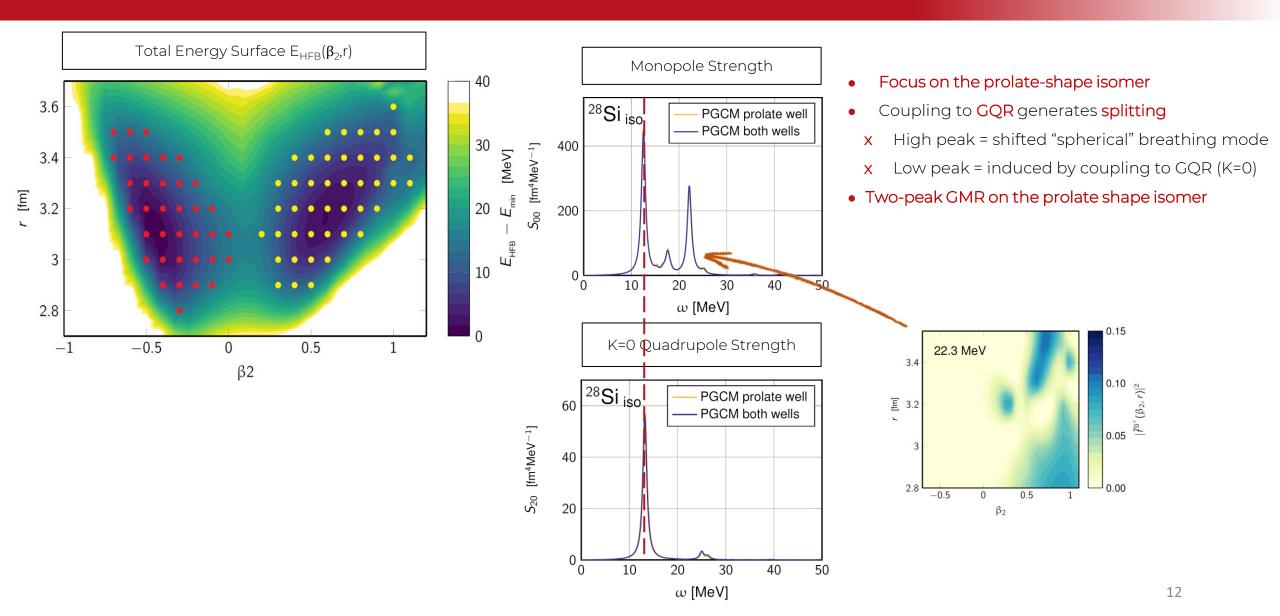


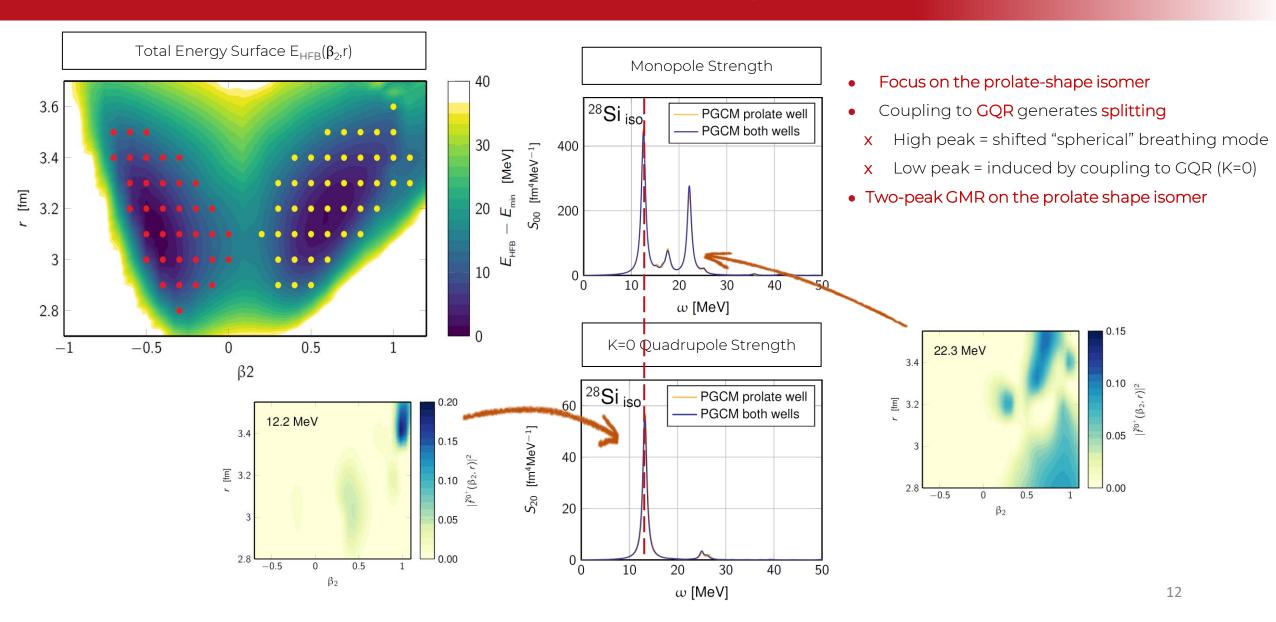
- Focus on the prolate-shape isomer
- Coupling to GQR generates splitting
 - X High peak = shifted "spherical" breathing mode
 - x Low peak = induced by coupling to GQR (K=0)

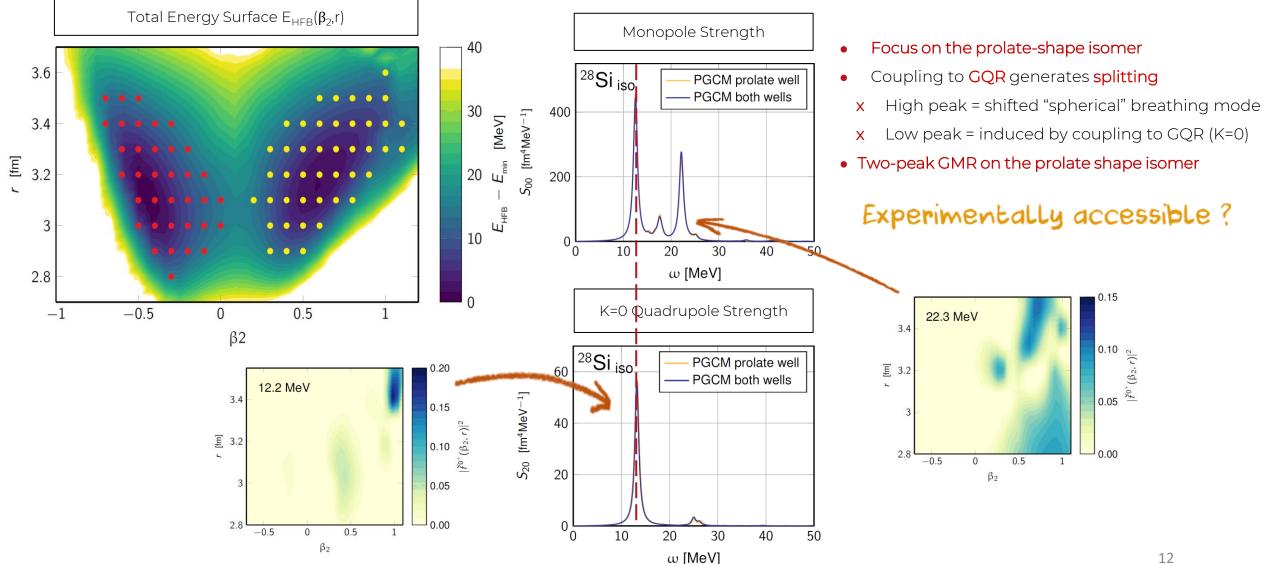




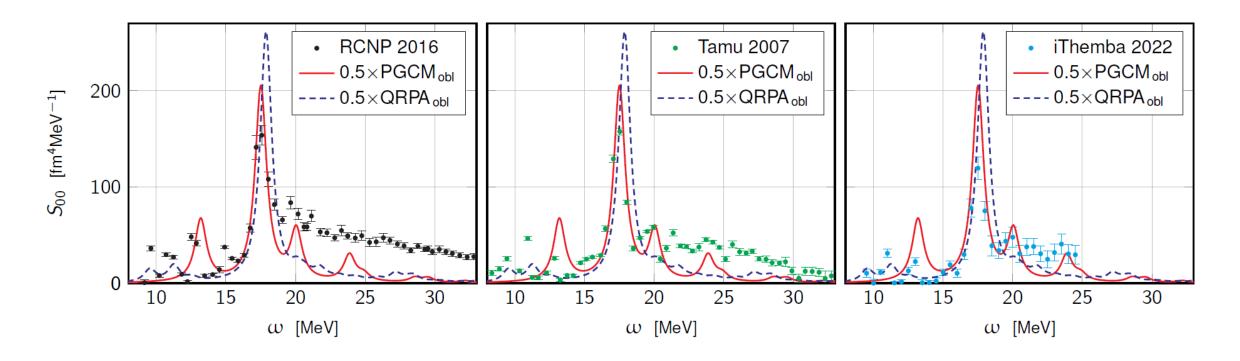








Comparison to experiment ²⁸Si



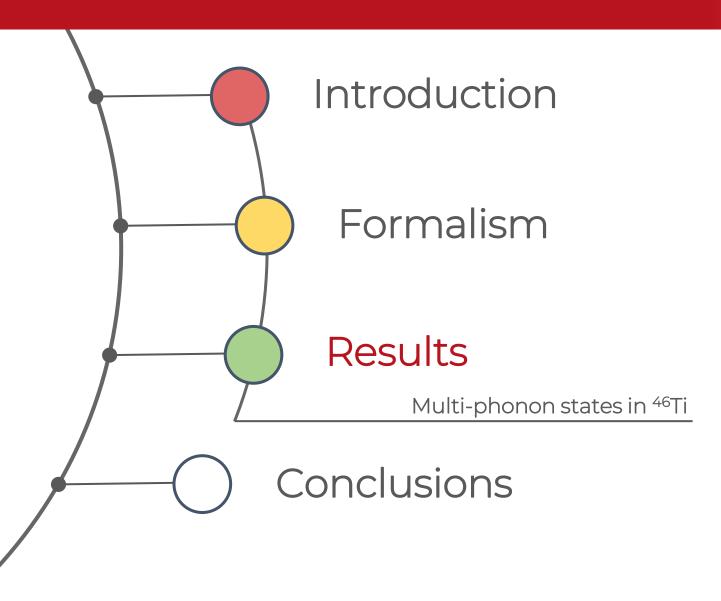
PGCM better reproduces the experimental data

- Better description of the main resonance
- Fragmentation effects are better captured than in QRPA

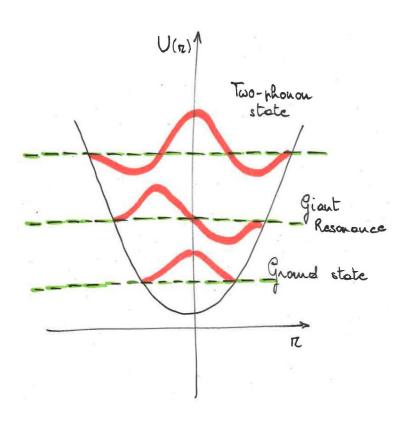
Experimental data are useful and promising to test different many-body methods

Data are not unambiguous, i.e. better resolution would be beneficial

Outline

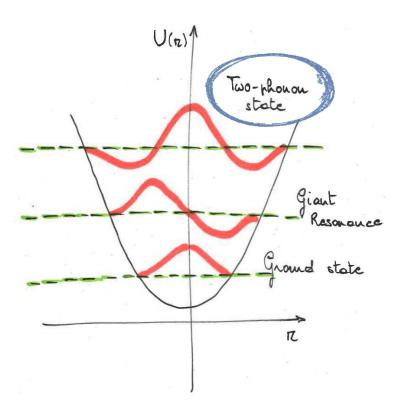


Multi-phonon states in 46Ti

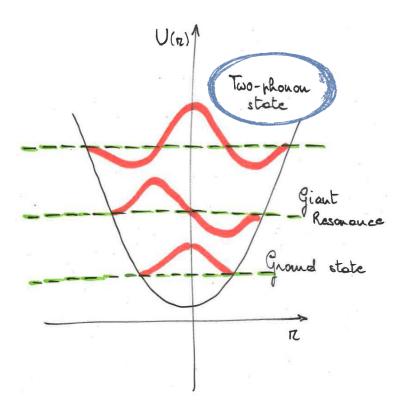


• GRs are the first phonon of a collective excitation

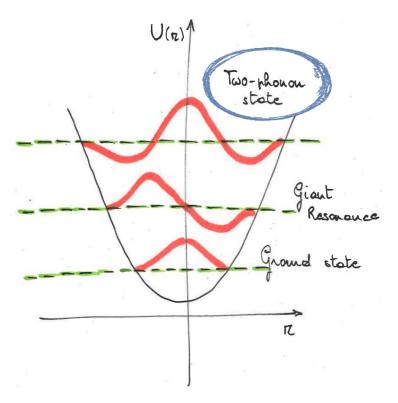
Multi-phonon states in 46Ti



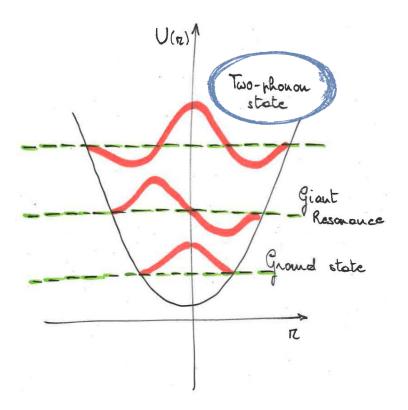
- GRs are the first phonon of a collective excitation
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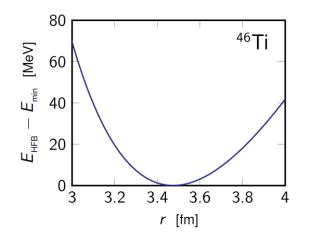


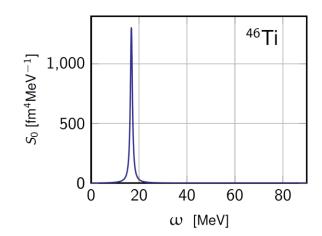
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- Not accessible to QRPA
- Equally spaced in the harmonic limit

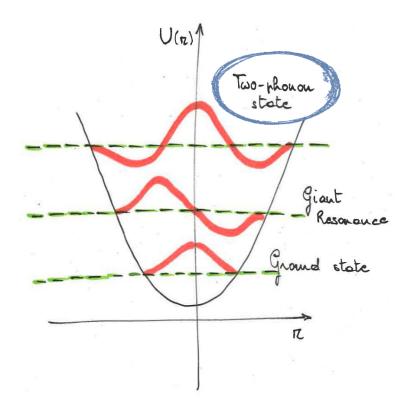


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One-dimensional PGCM calculation



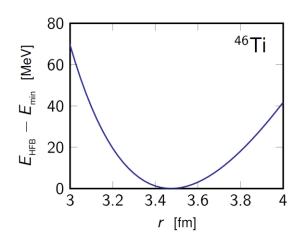


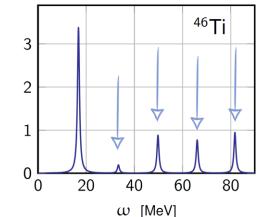


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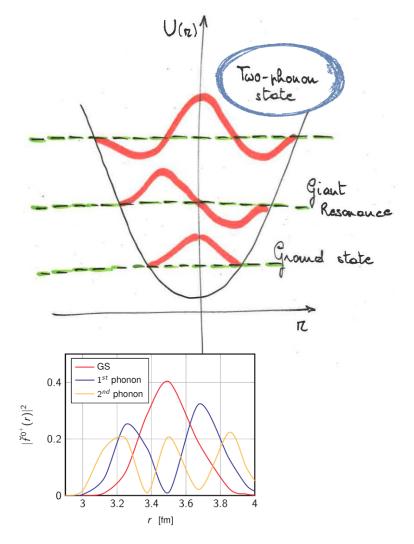
One-dimensional PGCM calculation

 $\log_{10} S_0 + 2$





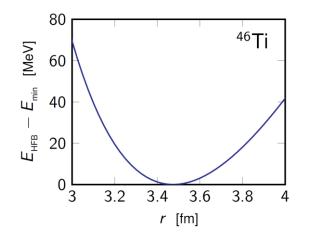
• PGCM predicts high-lying states

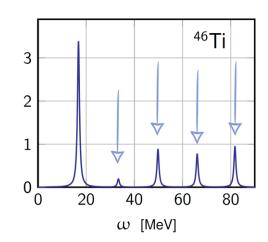


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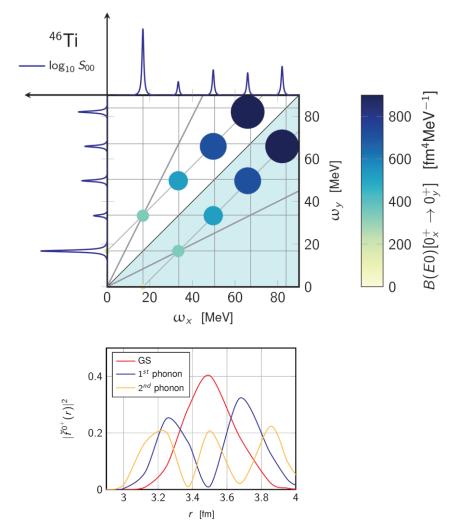
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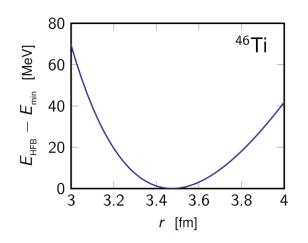
- PGCM predicts high-lying states
- Close to the harmonic oscillator eigen-solutions

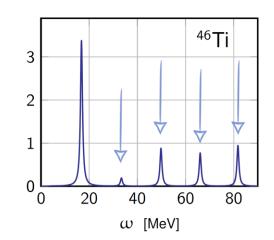


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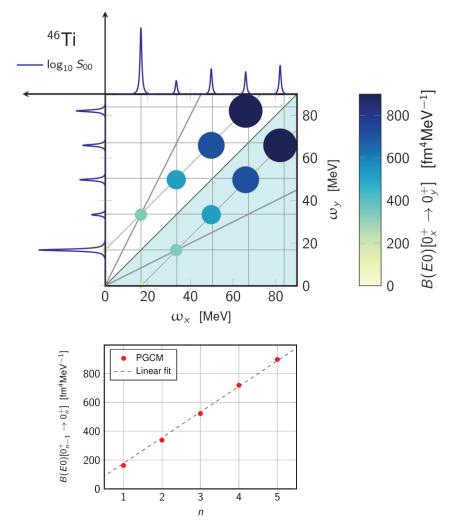
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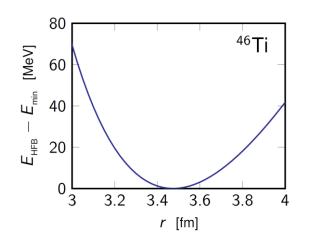
- PGCM predicts high-lying states
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- Transitions maximised between neighbouring phonons

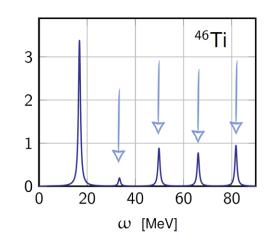


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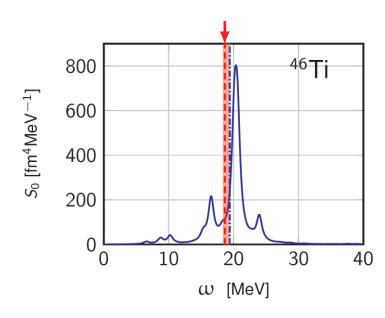
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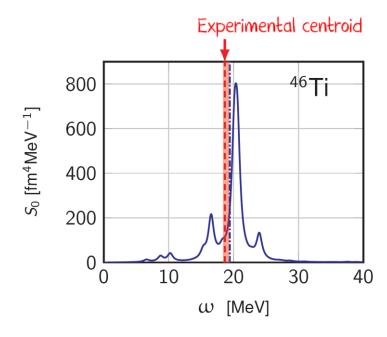




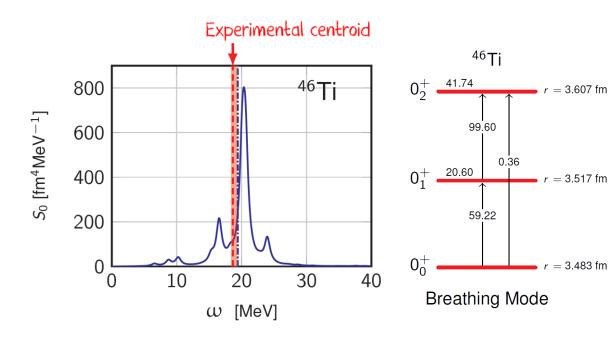
- PGCM predicts high-lying states
- Close to the harmonic oscillator eigen-solutions
- Transitions maximised between neighbouring phonons
- x Linear trend in the transition strength



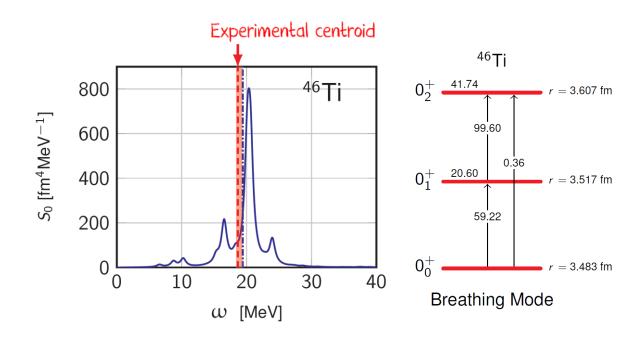
• Realistic PGCM in the (r, β_2) plane



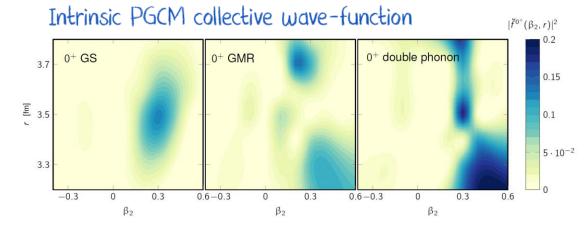
- Realistic PGCM in the (r, β_2) plane
- Good agreement with experiment

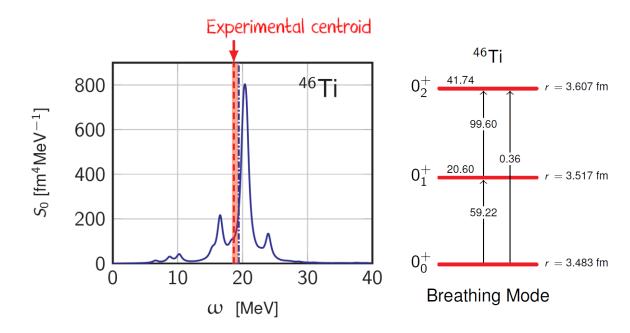


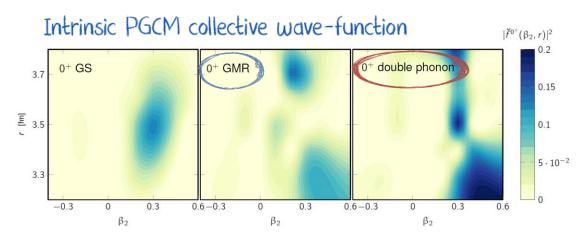
- Realistic PGCM in the (r, β_2) plane
- Good agreement with experiment
- Multi-phonon states observed



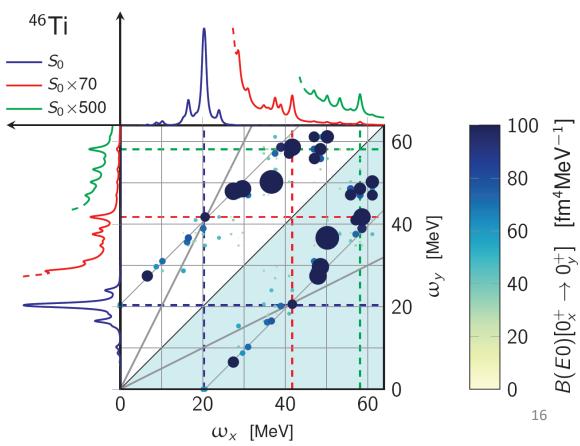
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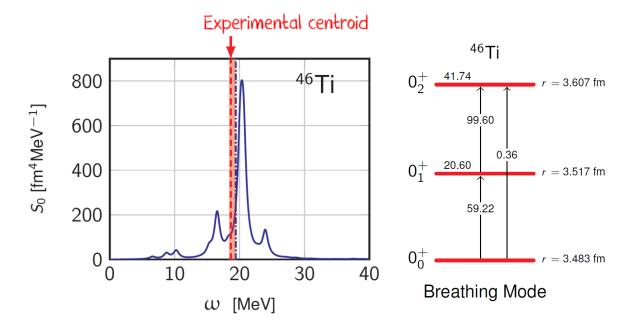


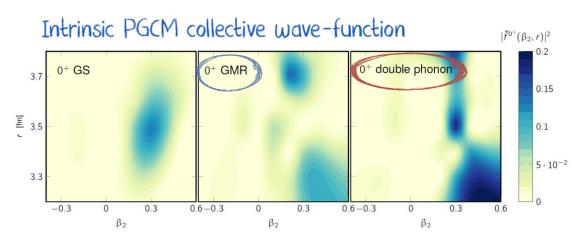




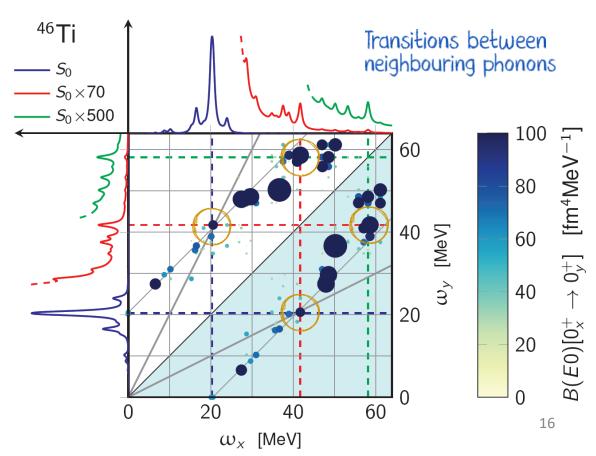
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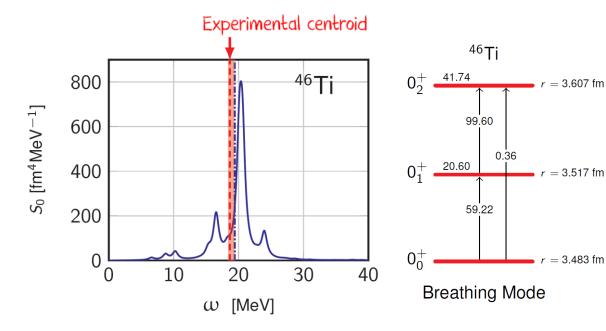


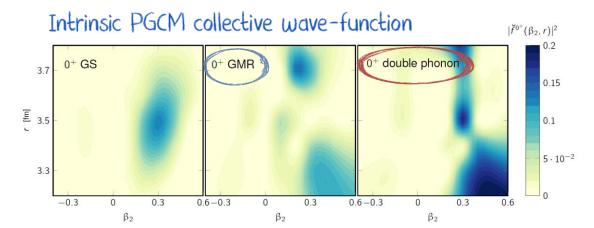




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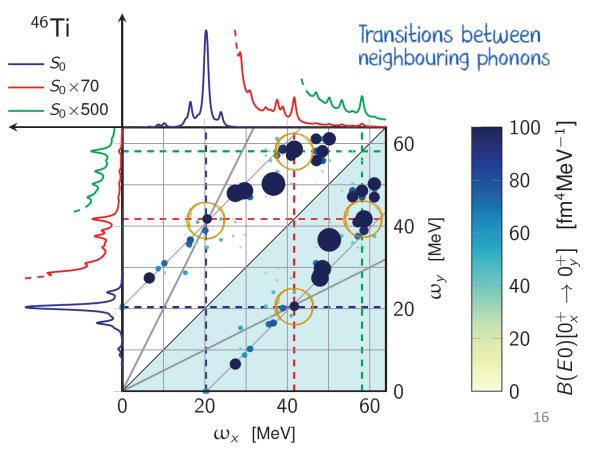




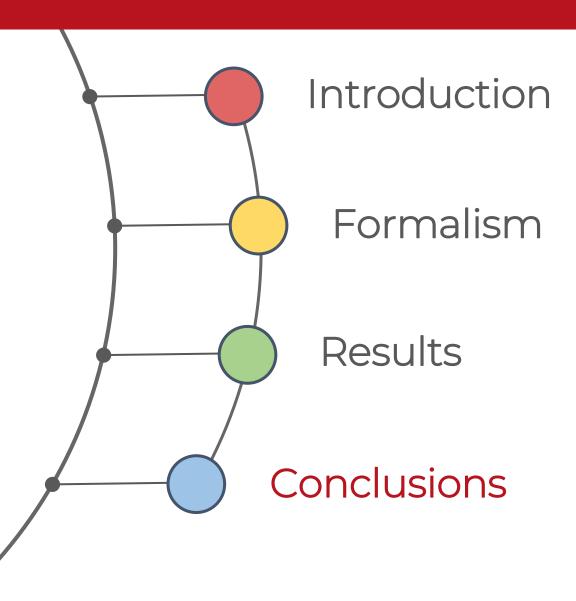


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Experimentally accessible?



Outline



PGCM is a valuable and reliable tool for *ab-initio* spectroscopy

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Different levels of symmetry breaking and restoration can reveal new physical and/or theoretical insights



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Access to observables and phenomena scarcely investigated previously in ab-initio

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Access to observables and phenomena scarcely investigated previously in ab-initio

What's next?

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Access to observables and phenomena scarcely investigated previously in ab-initio

What's next?

- Many upgrade concerning PGCM
 - Explore further generator coordinates
 - Deeper convergence sudy
 - Uncertainty quantification
 - Nuclear incompressibility

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Eigenvector Continuation



Develop full symmetry-conserving QRPA

[Federschmidt and Ring, NucPhysA, 1985]

Thanks for the attention



Thomas Duguet Vittorio Somà Benjamin Bally Alberto Scalesi



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Alexander Tichai



Pepijn Demol