Mean-Field and Beyond Mean-Field approaches for nuclear structure

Michael Bender (IP2I)

Marcella Grasso (IJCLab) & Nathalie Pillet (CEA DAM)

Atelier « Physique théorique des deux infinis »

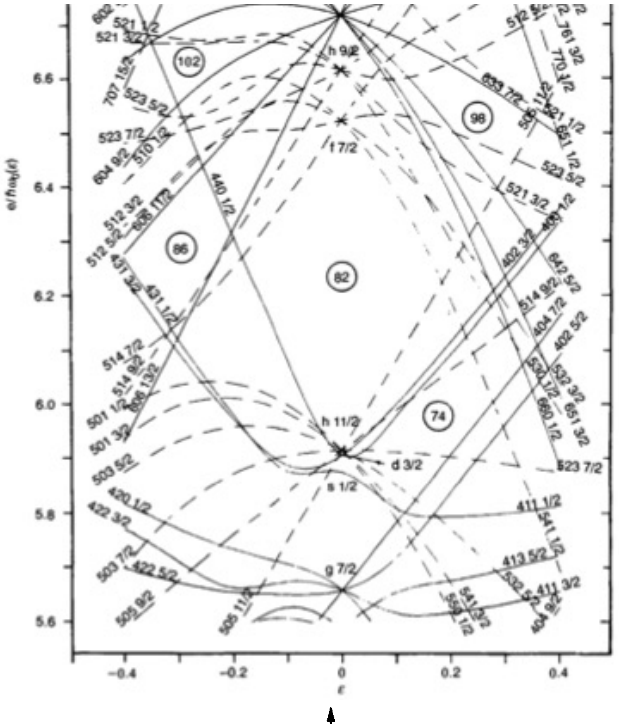
7-8 Juin 2021 en distanciel

The starting point: The self-consistent mean field

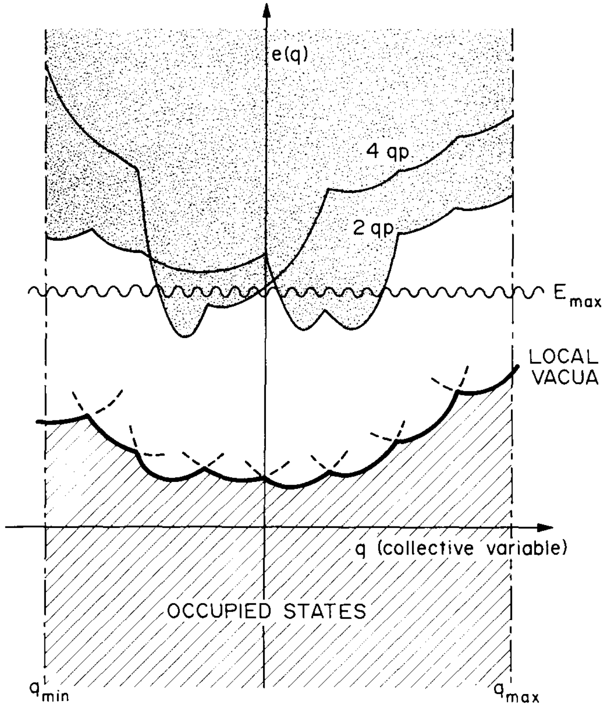
Variational principle

$$\delta E_{\psi} = 0 \quad \rightarrow \quad h\varphi = \boldsymbol{\varepsilon}\varphi$$

The total energy is calculated from a many product state $|\Psi>$, either directly as the expectation value of a Hamiltionian or indirectly as an energy density functional constructed from the one-body density matrices of such state.



- Energy-optimised single-particle states φ
- Brillouin's theorem: no coupling between ground state and 1p-1h excitations
- Lowest state might be symmetry breaking (deformation, pairing, …)
- Can be used to scan total energy as a function of « collective variables »
- Time-dependent variant can be linearised → RPA
- Starting point for « vertical » and « horizontal » expansions.



Dönau et al, NPA 496, 333 (1989).

Describing complex nuclear phénomena starting with simple states

Ongoing developments in France

- (Towards) symmetry-unrestriced self-consistent mean-field calculations

- Subtracted Second Random Phase Approximation (generalisation of of RPA in a vertical expansion)
- Multi-particle-multi-hole approach (configuration mixing in a vertical expansion optimising the reference)
- Symmetry-restored Generator Coordinate Method (configuration mixing in a horizontal expansion)

Related topics not covered here:

- Need for generalised (effective) interactions (talk by Marcella Grasso)
- Need for improved and/or specific fit protocols (talk by Marcella Grasso)
- Improved explicit time evolution (talk by David Regnier)

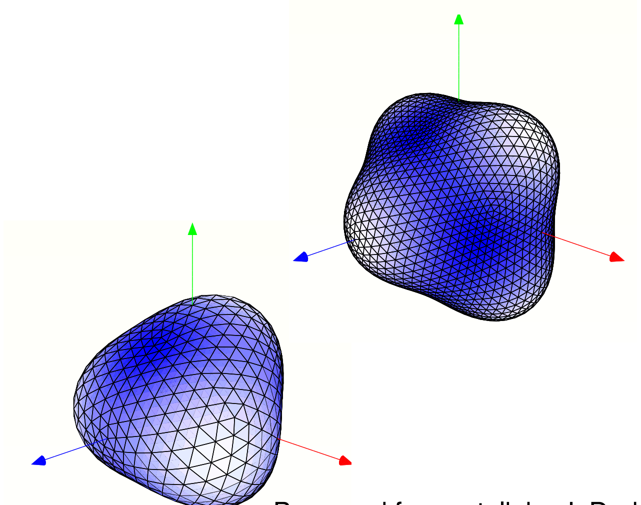
Symmetry-unrestricted self-consistent mean fields for complex and exotic configurations of nuclei

Physics cases:

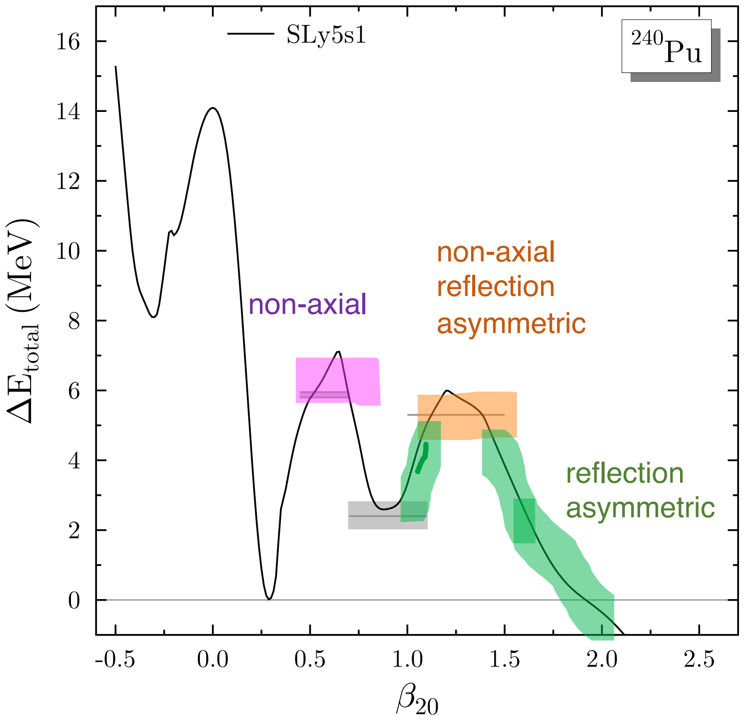
- Exotic shapes dominated by high multipoles
- Fission paths
- Relative orientation of the collective angular momentum, angular momenta of single-particle states and the shape

Codes are more difficult to set up and run:

- Often multi-constrainted calculations needed
- Additional constraints needed to fix center of mass and relative orientations
- Often soft directions in the energy surface

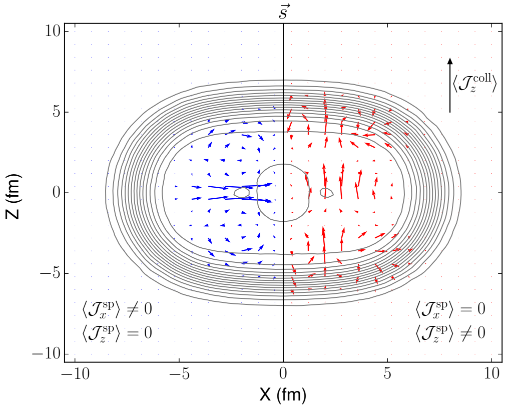


Borrowed from a talk by J. Dudek

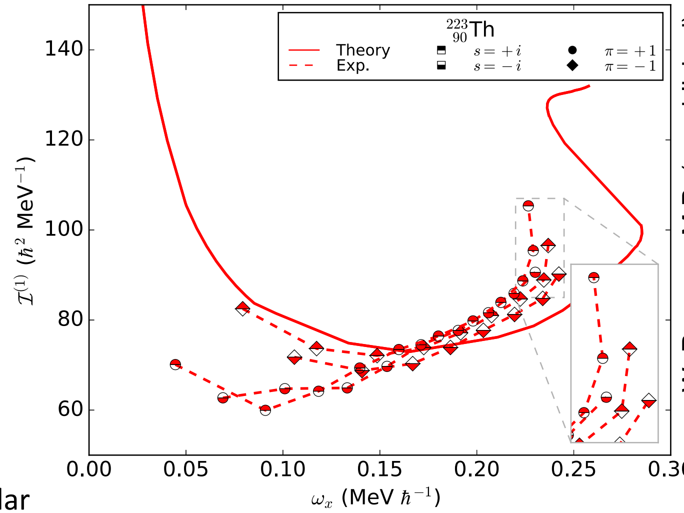


W. Ryssens, M. Bender, K. Bennaceur, P.-H. Heenen, J. Meyer, PRC99 (2019) 044306

W. Ryssens, M. B. (unpublished)



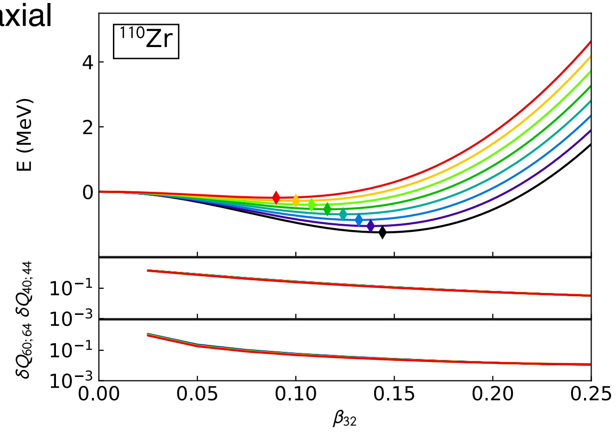
Spin distribution is different when choosing angular momentum to be aligned with the long axis or a short one.



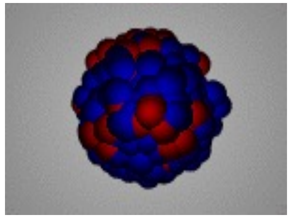
W. Ryssens, M.B. (unpublished)

moment of inertia from cranked HFB of an odd octupole-deformed nucleus.

softness against non-axial octupole deformation depends on the parameterisation of the EDF!



W. Ryssens, M. Bender, K. Bennaceur, P.-H. Heenen, J. Meyer, PRC99 (2019) 044306



THE SSRPA MODEL M. Grasso in collaboration with D. Gambacurta (LNS, Catania)

What we want to describe: excitation spectra in a many-body system.

Important experimental program in France and all over the world for measuring charge-conserving and charge-exchange excitations in nuclei

Mean-field : only individual degrees of freedom → Adding fluctuations to the self-energy generated by particle-hole bubbles (random-phase approximation)

… but not enough to describe **widths and strength fragmentation** of collective modes.

NEED TO GO BEYOND!!!

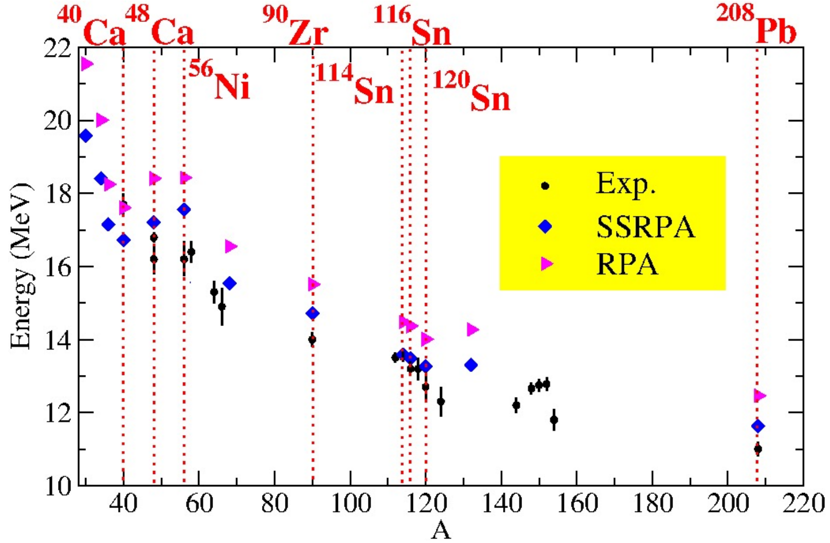
How: subtracted second random-phase approximation (SSRPA)-> **two particle-two hole (2p2h) configurations included in the excitation operators.**

The self-energy becomes energy dependent and incorporates beyond-mean-field effects (individual degrees of freedom couples with 2p2h configurations). Subtraction procedure for handling double-counted correlations

-> state-of-the-art model for predicting excitation spectra

$$Q_\nu^\dagger = \sum_{ph} \left(X^\nu_{ph} a_p^\dagger a_h - Y^\nu_{ph} a_h^\dagger a_p \right) + \sum_{p<p',h<h'} \left(X^\nu_{php'h'} a_p^\dagger a_h a_{p'}^\dagger a_{h'} - Y^\nu_{php'h'} a_h^\dagger a_p a_{h'}^\dagger a_{p'} \right)$$

Heavy numerical problem, unaffordable up to one decade ago (strong cuts and approximations were done)



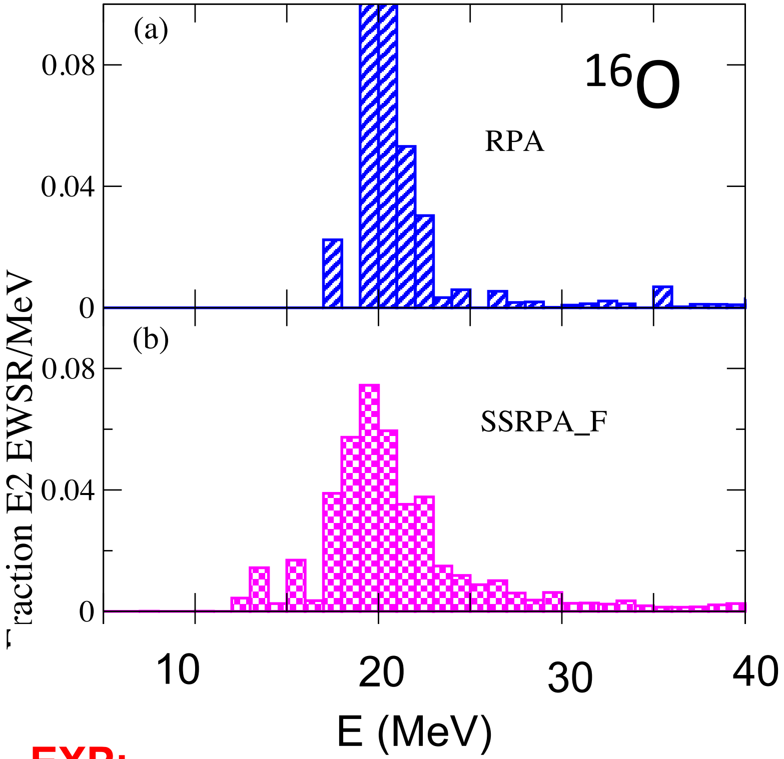
Centroids of Isoscalar GQRs from ^{30}Si to ^{208}Pb

Vasseur, Gambacurta, Grasso, PRC 98, 044313 (2018)

Spreading width of quadrupole excitations.

Centroid: 20.73 MeV
Width: 2.42 MeV

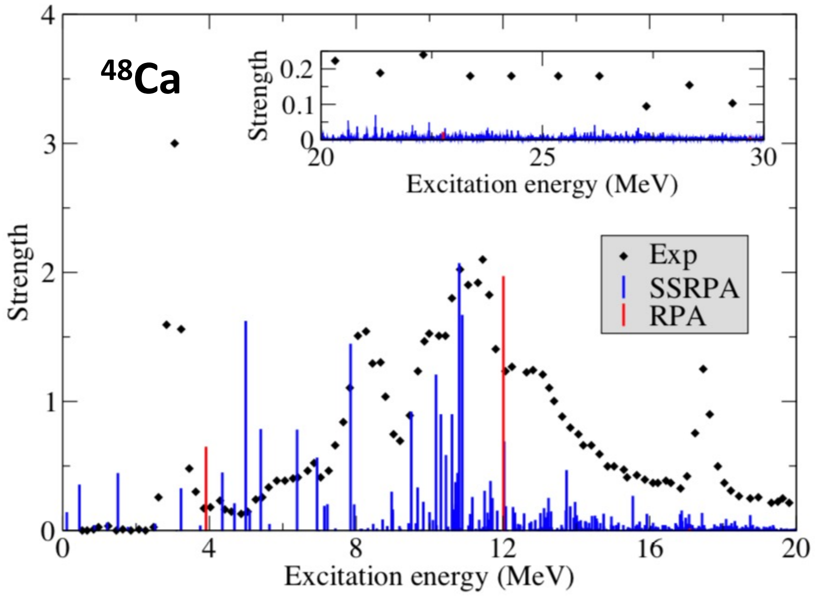
Centroid: 20.21 MeV
Width: 4.05 MeV



EXP:
Centroid: 19.76 MeV
Width: 5.11 MeV

Calc: Gambacurta, Grasso, Engel, PRC 92, 034303 (2015)

Expt: Lui, Clark, Youngblood, PRC 64, 064308 (2001)



The mystery of the missing GT strength: 2p2h configurations have a density that increases with the excitation energy. This pushes an important amount of strength to high energy

Gambacurta, Grasso, Engel, PRL 125, 212501 (2020)

Globally: better agreement with the experimental data compared to RPA

Impact: some recent work

◆ **Electric dipole polarizability in ^{48}Ca,**
Gambacurta, Grasso, Vasseur, Phys Lett. B 777, 163 (2018)

◆ **Systematic study of axial compression modes,**
Vasseur, Gambacurta, Grasso, Phys Rev C 98, 044313 (2018)

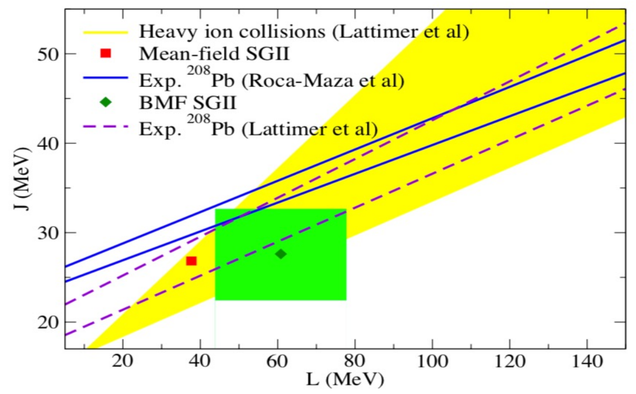
◆ **Beyond-mean-field effects on effective masses,**
Grasso, Gambacurta, Vasseur, Phys Rev C 98, 051303(R) (2018)

◆ **Beyond-mean-field effects on the symmertry energy and its slope from the low-lying dipole response of ^{68}Ni,**
Grasso and Gambacurta, Phys. Rev. C 101, 064314 (2020)

◆ **Gamow-Teller strengths in ^{48}Ca and ^{78}Ni with the charge-exchange subtracted second random-phase approximation,**
Gambacurta, Grasso, Engel, Phys. Rev. Lett. 125, 212501 (2020)

◆ **Soft compression modes and links with the incompressibility of asymmetric matter,** Gambacurta, Grasso, Sorlin, Phys Rev C 100, 014317 (2019)

Beyond-mean-field effects on infinite matter properties



Well-established interactions with experimentalists.

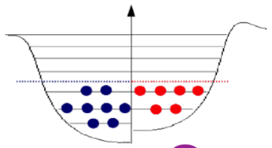
Important achievement
- For the community working on charge-exchange excitations: starting now systematic applications
- Towards the computation of nuclear matrix elements for neutrinoless double beta decay (see talk by F. Nowacki)

Multi-particle-multi-hole approach

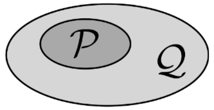
Truncated Hilbert space

- Trial wave function : Superposition of Slater determinants

$$|\Psi\rangle = A_{0p0h}|\Phi_{0p0h}\rangle + \sum_{1p1h} A_{1p1h}|\Phi_{1p1h}\rangle + \sum_{2p2h} A_{2p2h}|\Phi_{2p2h}\rangle + \sum_{3p3h} A_{3p3h}|\Phi_{3p3h}\rangle + \ldots$$



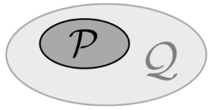
$$|\Phi_{0p0h}\rangle = \prod_i a_i^\dagger |0\rangle$$



- Advantages : Symmetry preservation (particle numbers, rotational invariance, Pauli principle, ...)
- Applicable to even-even, odd and odd-odd nuclei
- Diagonalization of the Hamiltonian in the N-body space P

$$\delta\mathcal{E}[\Psi]_{/\{A^*_\alpha\}} = 0 \;\Rightarrow\; \sum_\beta A_\beta \langle\phi_\alpha|\hat{H}|\phi_\beta\rangle = E A_\alpha$$

$$\begin{pmatrix} H_{PP} & H_{PQ} \\ H_{QP} & H_{QQ} \end{pmatrix} \Longrightarrow \begin{pmatrix} H_{PP} & H_{PQ} \\ H_{QP} & H_{QQ} \end{pmatrix}$$

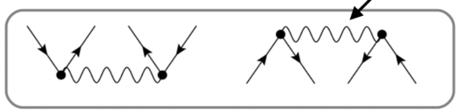


=> All types of correlations (static and dynamical ones) :

Excitation order of the configuration

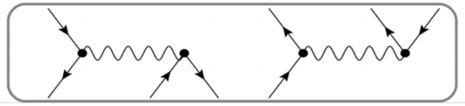
Interaction vertex $\langle\phi_\alpha|\hat{V}|\phi_\beta\rangle$

$|n_\alpha - n_\beta| = 2$



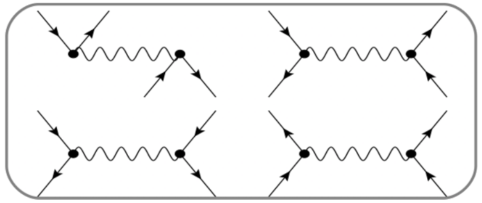
RPA, pairing

$|n_\alpha - n_\beta| = 1$



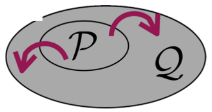
Particle-vibration coupling

$|n_\alpha - n_\beta| = 0$



RPA

Pairing



- Optimization of the orbitals consistently with the N-body correlations in P+Q space

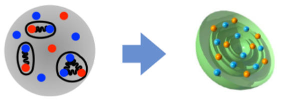
$$\delta\mathcal{E}[\Psi]_{/\{\varphi^*_i\}} = \langle\Psi|\left[\hat{H},\hat{T}\right]|\Psi\rangle = 0 \;\Leftrightarrow\; \left[\hat{h}(\rho),\hat{\rho}\right] = \hat{G}(\sigma)$$

"Generalized Brillouin equation"

Generalized mean-field equation

- Building of a generalized mean-field in a N-body space

(equivalent to solving a Dyson equation)



- Interactions : MPMH approach usable with both bare and effective interactions (talk M. Grasso)

Future developments

Formal developments :

- Building of the Hessian matrix : Are there situations in which the variations according to {A} and {ϕ} are correlated?
- (short range versus long range correlations)
- MPMH renormalized operators (effective operators)
- Input for nuclear reaction models and building of an optical potential (see talk by G. Hupin)

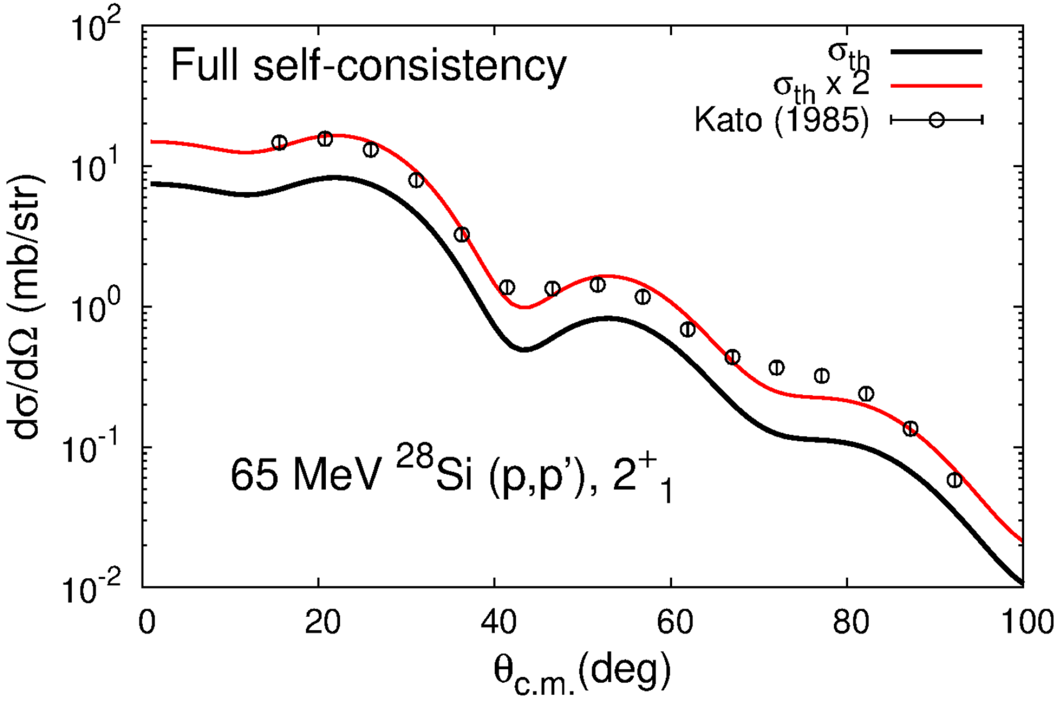
Numerical challenges :

- Going to heavy nuclei
- Porting to HPC in the era of exascale computing
- Efficient truncation schemes / role of meta-modeling and AI (see talk by G. Hupin)

Examples of physics cases :

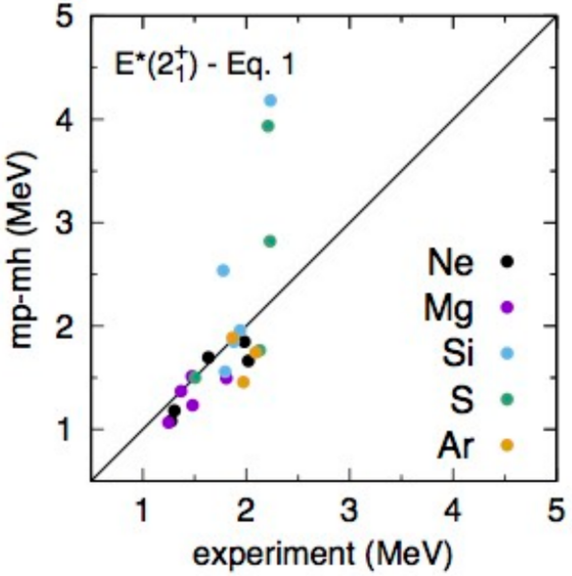
- Low-energy spectroscopy of stable and exotic nuclei
- Evolution of shell closures and their signatures
- Proton-neutron pairing correlations
- Multipolar resonances and electro-weak transitions
- Halos, triton and alpha clustering in light nuclei (quantum entanglement)
- …

(mixing in the sd-shell only, Gogny D1S)

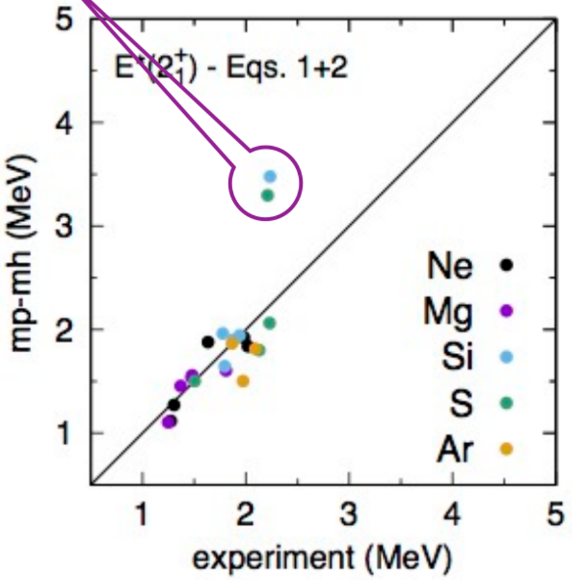


Example : Orbital optimization effect on excitation energies

T=0 component of the Gogny force
(lack of tensor term, *Pillet et al. PRC 85, 044315 (2012)*)



Orbital optimization



All
$$\langle \Delta E^* \rangle = 373 \text{ keV}$$
$$\sigma(\Delta E^*) = 517 \text{ keV}$$

^{30}S & ^{30}Si excluded
$$\langle \Delta E^* \rangle = 226 \text{keV}$$
$$\sigma(\Delta E^*) = 214 \text{ keV}$$

All
$$\langle \Delta E^* \rangle = 235 \text{ keV}$$
$$\sigma(\Delta E^*) = 323 \text{ keV}$$

^{30}S & ^{30}Si excluded
$$\langle \Delta E^* \rangle = 142 \text{ keV}$$
$$\sigma(\Delta E^*) = 122 \text{ keV}$$

C. Robin, N. Pillet, D. Pena Artega, J.-F. Berger, PRC 93 (2016) 024302.
C. Robin, N. Pillet, M. Dupuis, J. Le Bloas, D. Pena Artega, J.-F. Berger, P¨RC 95 (2017) 044315.

Symmetry-restored Generator Coordinate Method

Toolbox that can be used in many different contexts and that can be embedded into many frameworks:

- MR-EDF (beyond the symmetry-breaking self-consistent mean-field)
- Valence-space Hamiltonians (filter to target specific excitations in shell-model calculations)
- Ab-initio methods of various flavours

Projection (on particle number, angular momentum, parity, isospin, center-of-mass momentum, …)

$$\left|\Psi_{\epsilon}^{\lambda i}\right\rangle = \sum_{j=1}^{d_\lambda} f_{\epsilon}^{\lambda j}\, \hat{P}_{ij}^{\lambda}\, |\Theta\rangle, \qquad \boldsymbol{H}^{\lambda}\, \boldsymbol{f}_{\epsilon}^{\lambda} = e_{\epsilon}^{\lambda}\, \boldsymbol{N}^{\lambda}\, \boldsymbol{f}_{\epsilon}^{\lambda},$$

see B. Bally & M. Bender, PRC103 (2021) 924315 for everything you always wanted to know about projection but were afraid to ask.

Refined description of of nuclear structure and reactions:

- Additional correlations not grasped by symmetry breaking
- Restoration of selection rules for electromagnetic, weak, … transitions

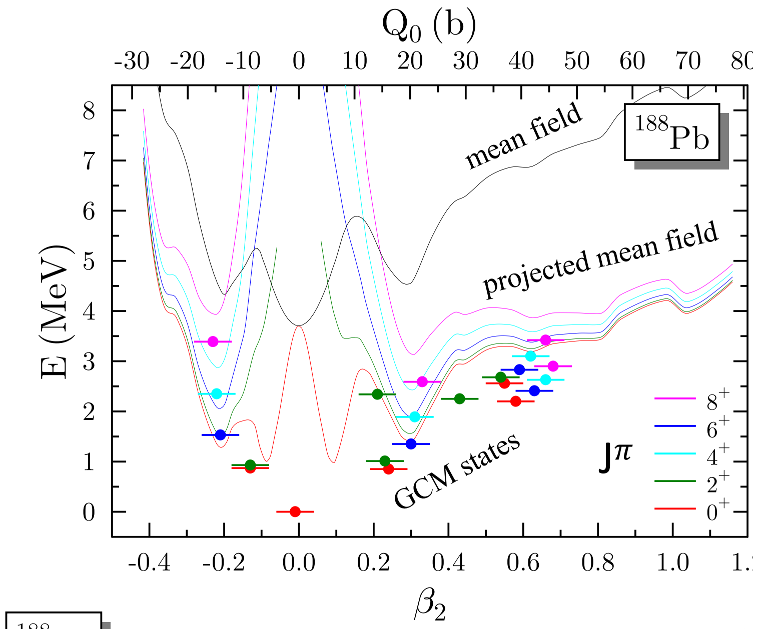
Generator Coordinate Method

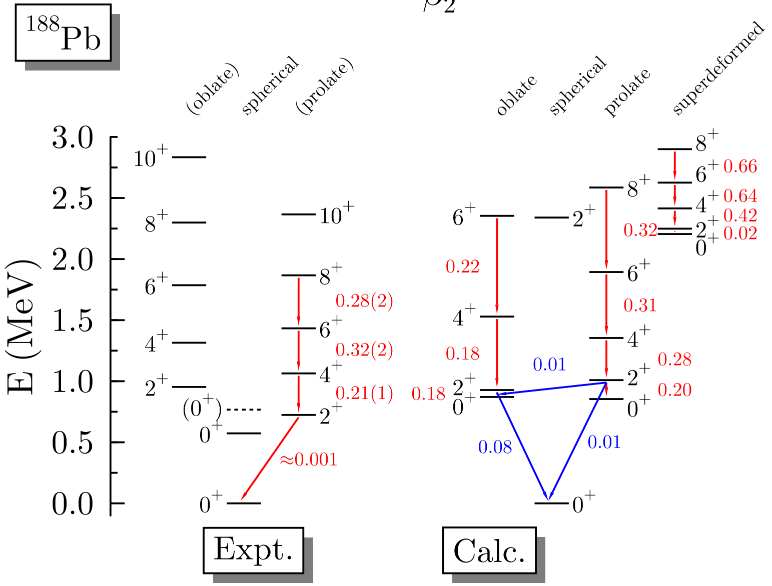
$$|\Phi_E^{\lambda i}\rangle = \sum_q f_{q,E}^{\lambda i}\, |\Psi^{\lambda i}(q)\rangle$$

see M. Bender, N. Schunck, J. P. Ebran, T. Duguet, Chapter 3 of N. Schunck (ed.) Energy Density Functionals for Atomic Nuclei, IOP (2019).

- Configuration mixing of non-orthogonal states (shapes, angular momenta, intensity of pairing, …)

Shape coexistence & mixing

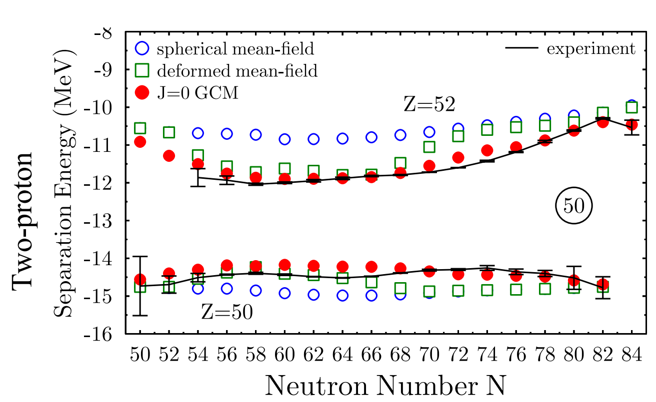




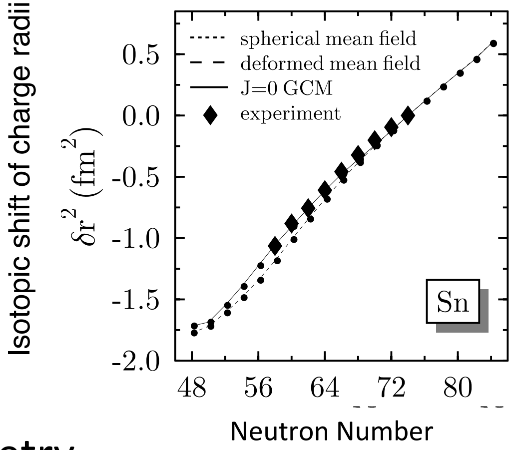
numbers in colour are dimensionless transition quadrupole moments

adapted from M. Bender, P. Bonche, T. Duguet, P.-H. Heenen, PRC 69 (2004) 064303

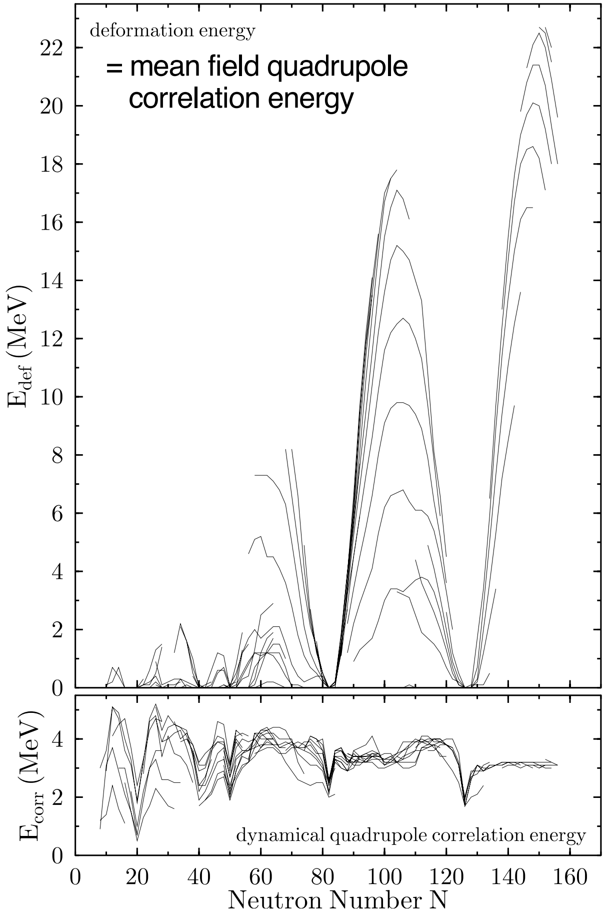
Ground-state correlations



BBH, PRC 789 (2008) 054312



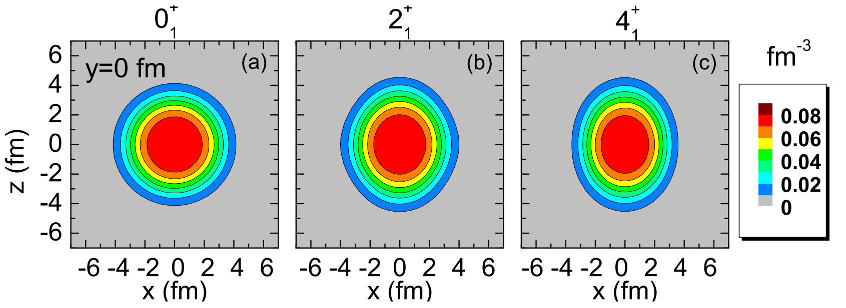
BBH, PRC73 (2006) 034322



M. Bender, G.F.Bertsch, P.-H. Heenen, PRC73 (2006) 034322

Revelant for

- mass spectrometry
- prompt gamma-ray spectroscopy
- decay spectroscopy
- laser spectroscopy
- electron scattering
- Coulomb excitation
- ….



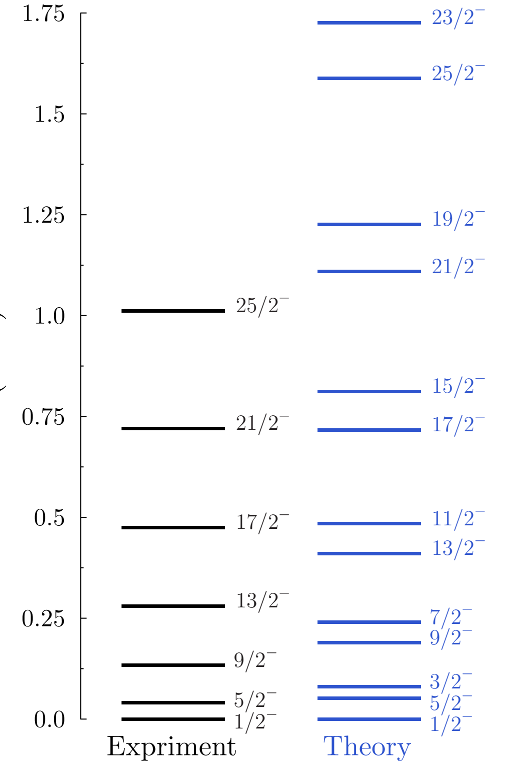
density distribution of projected states in the laboratory frame

Yao, Bender, Heenen, PRC 91 (2015) 024301

MR EDF of SHE

Projected GCM as an approximation to CI

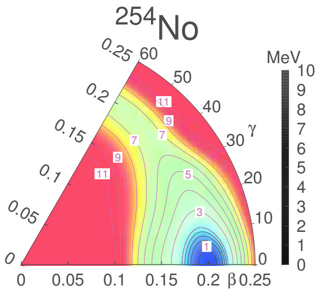
(see also talk by K. Sieja)



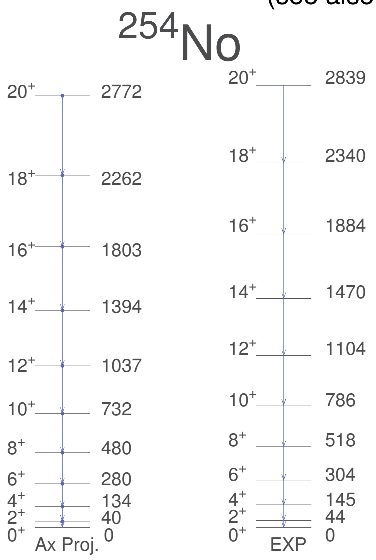
From 1qp: $K^{\pi} = 1/2^{-}$

Heenen, Bally, Bender, Ryssens, EPJWC131 (2016) 02001

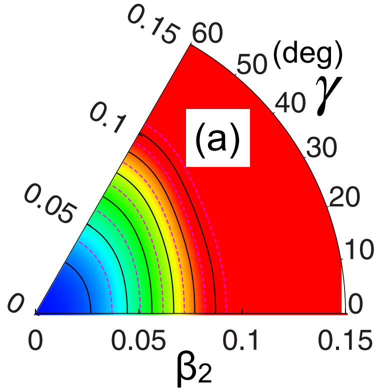
J	rrmsp (fm)	rrmsn (fm)	mu (mu_N)	Q_s e fm^2
7/2	5.8769	6.0193	1.4540	596.84
9/2	5.8769	6.0194	1.8407	232.67
11/2	5.8769	6.0194	2.2308	14.27
13/2	5.8769	6.0194	2.6230	-127.63
15/2	5.8770	6.0194	3.0164	-225.40
17/2	5.8770	6.0195	3.4108	-295.86
19/2	5.8771	6.0195	3.8057	-348.48
21/2	5.8771	6.0196	4.2011	-388.91
23/2	5.8772	6.0196	4.5968	-420.74
25/2	5.8773	6.0197	4.9928	-446.29

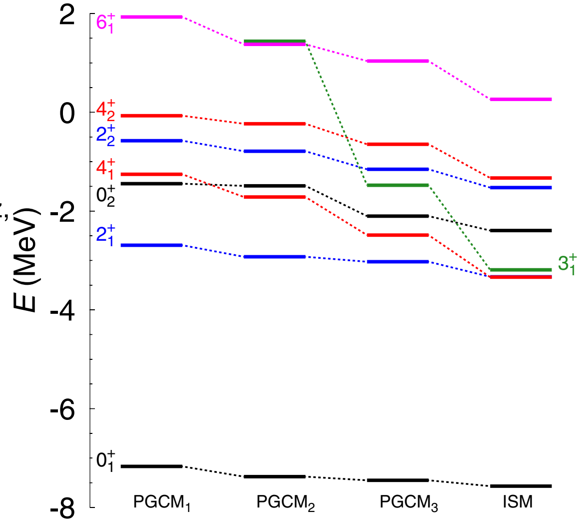


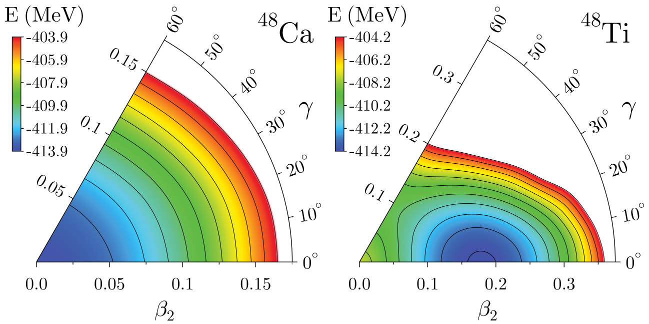
Bouthong, thesis Strasbourg (2016)

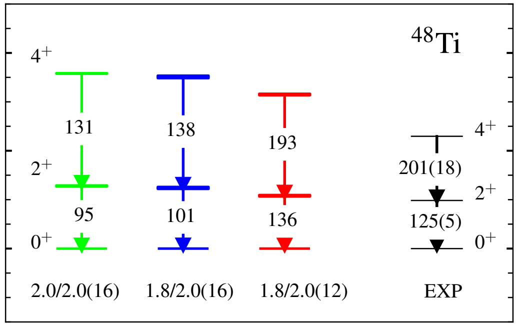


Bally, Sanchez-Fernandez, Rodriguez, PRC 100 (2019) 044308





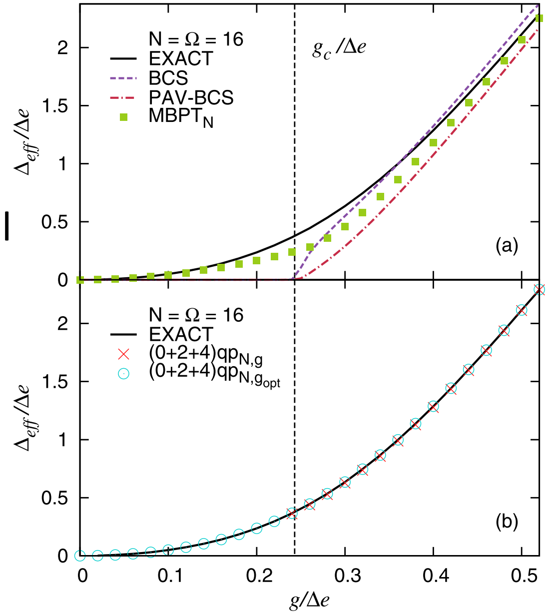




Ab-initio:
In-medium SRG

Yao, Bally, Engel, Wirth, Rodriguez, Hergert, PRL 124, 232501 (2020)

Combining vertical and horizontal expansions



Ripoche, Lacroix, Gambacurta, Ebran, Duguet, PRC95 (2017) 014326

Summary & Outlook

Mean field:

- Towards symmetry-unrestricted self-consistent mean-field describe the complex geometrical arrangement of nucleons (shape and direction of angular momentum).

Beyond the mean field:

- Three complementary directions to go « beyond the mean field » explored by the french community: vertical, vertical + feedback from horizontal, horizontal (with optional bits of vertical)
- These approaches target different phenomena, but have overlapping validity ranges.
- Choice of many-body technique and the effective energy density functional / Hamiltonian is intertwined.

Overall aims and scopes:

- Refined description of of nuclear structure and reactions.
- Better microscopic understanding of nuclear phenomena.
- Interactions with, and support for, the community of experimentalists.

Following these routes requires (and is made possible by) high-performance computing.

But don't forget that we need suitable Hamiltonians and/or energy density functionals for these techniques!