Beyond mean field in nuclear structure: symmetry restoration and configuration mixing

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Everybody in the audience knows pretty well the characteristics of the Gogny interaction ....

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... and how nicely describes many nuclear properties like binding energies, radii, quadrupole moments, moments of inertia, fision barrier heights...

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... using the mean field theoretical framework (HFB) and only one parametrization of the force (D1S, 1984) valid all over the Nuclide chart ...

Beyond mean field

but the Gogny force was devised not only to be used at the mean field level but also to be used together with "beyond mean field" methods.

- Beyond but not too far away meand field methods
  1. RPA
  2. GCM+GOA $\rightarrow$ "Collective Schrodinger Equation"
  3. ZPE as "fluctuation" over "collective mass"
- Traditional beyond mean field methods
  1. Exact restoration of broken symmetries
  2. Full GCM

Beyond mean field

There are good reasons to go beyond mean field

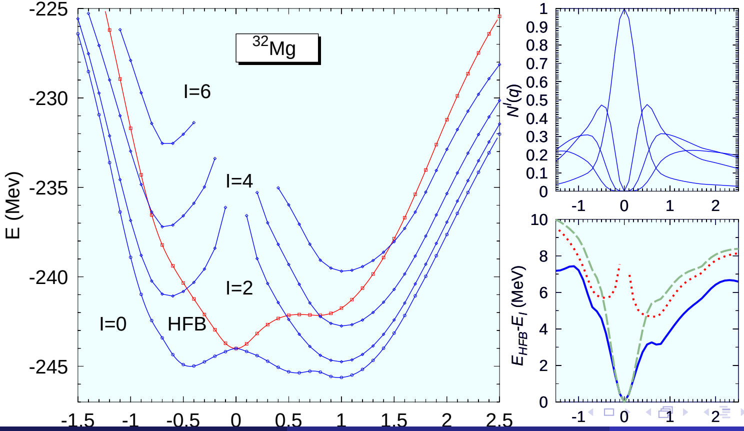
- Broken symmetries have to be properly restored to have wave functions with the necessary symmetry properties: this might not be relevant for scalar quantities like energies, radii, etc but it is fundamental to compute transition probabilities (selection rules, etc)
- Correlations associated to symmetry restoration and/or fluctuations in relevant symmetry-breaking parameters (for instance $\langle \Delta N^2 \rangle$ in particle number symmetry) can affect the nuclear dynamics.
  This is specially true for particle number restoration as the level density around the Fermi surface if quite strongly affected by PNP.
- As more nuclear species are being studied in detail experimentally it is becoming clear that situations where two coexisting configurations strongly interact are not as exceptional as thought before (neutron deficient lead isotopes, neutron rich magnesium isotopes,etc)

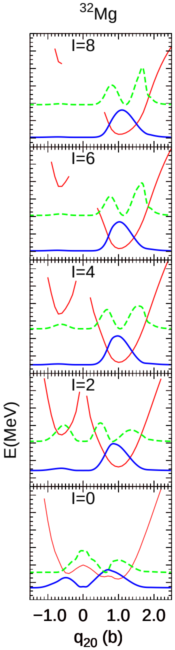
^{32}Mg

- Experimentally, it has been quite unambiguously established that its ground state is quadrupole deformed
- With all the reasonable parameterizations of the Skyrme interaction and the relativistic mean fields as well as with the three parametrizations of the Gogny interaction the ground state obtained in the mean field calculations is spherical at the mean field level
- Only after considering angular momentum projection a quadrupole deformed ground state is obtained
- The prolate quadrupole deformed ground state coexist with an oblate configuration and configuration mixing with the quadrupole degree of freedom as collective coordinate strongly affect the theoretical predictions and therefore can not be disregarded.

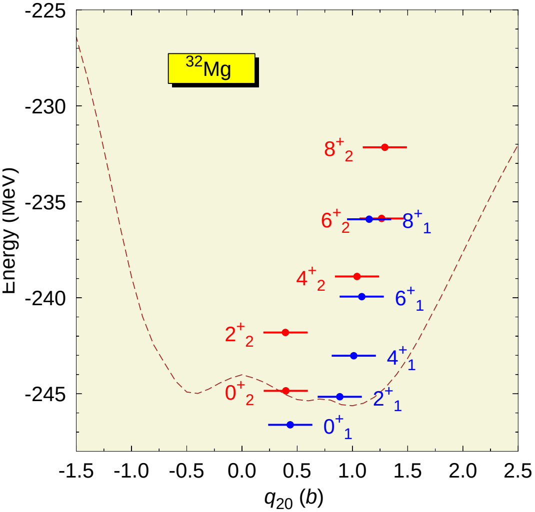
^{32}Mg

Gogny interaction D1S + Angular Momentum Projection

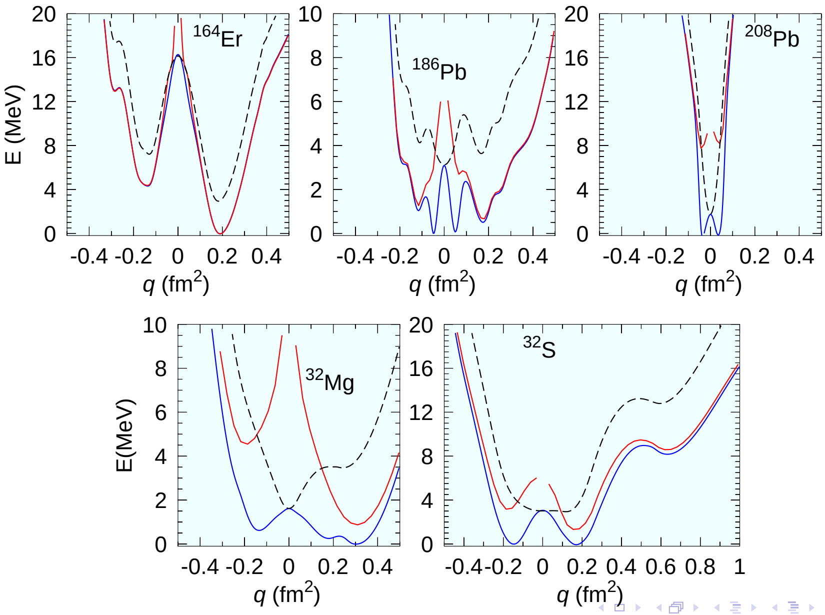




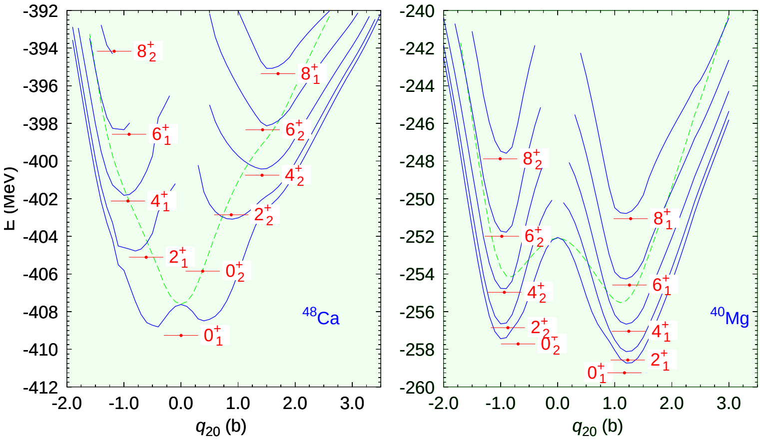
	GCM	AMP	EXP
$\Delta E_{0^+-2^+}$	1.46	0.87	0.88
$B(E2, 0^+ \to 2^+)$	395	593	454 ± 78



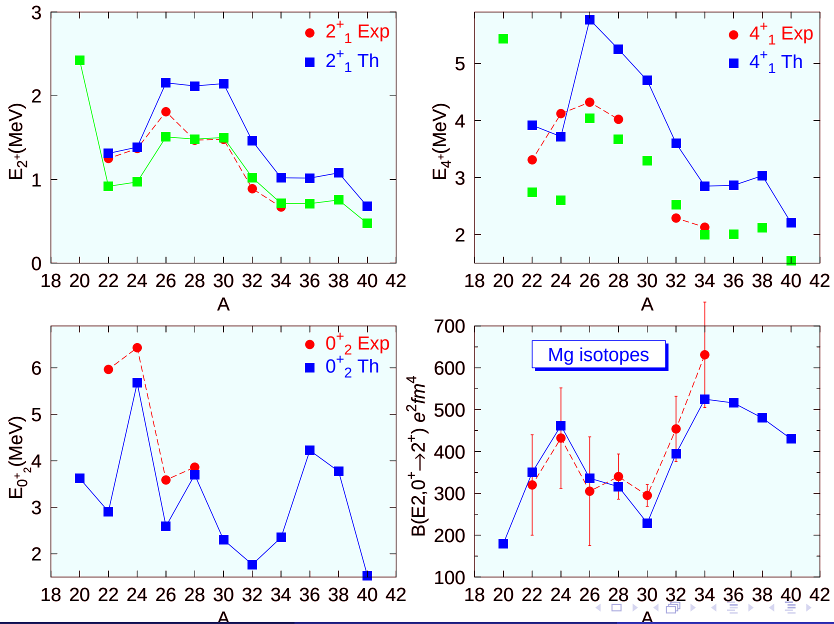
more examples of AMP



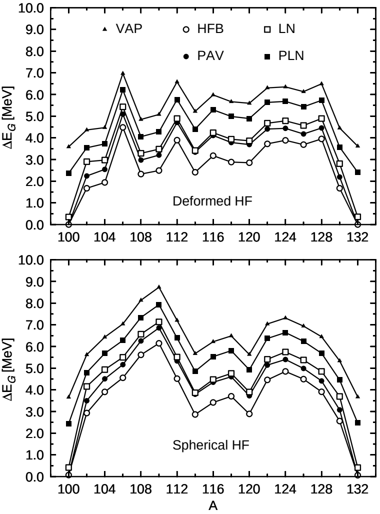
Spherical and Deformed nuclei



Mg istopic chain



Particle number projection



Pairing correlations in the Tin isotopes
Comparison of theoretical approache

What to do next ...

- Triaxial AMP
- AMP in odd-A systems
- AMP for 2qp, 4qp, etc
- + PNP
- + Parity
- + PBV
- ....

but, unfortunately, life is not easy ....
and we have to solve first some "technical details" ...

Some technicalities

In the GCM and projection one has to deal with linear combinations of mean field wave functions (HF or HFB) $|\Phi(q)\rangle$

$$|\Psi\rangle = \int dq f(q)|\Phi(q)\rangle$$

$$E = \frac{\langle\Psi|H|\Psi\rangle}{\langle\Psi|\Psi\rangle} = \frac{\int dqdq' f^*(q) f(q') \mathcal{H}(q,q')}{\int dqdq' f^*(q) f(q') \mathcal{N}(q,q')}$$

Hamiltonian and norm overlaps

$$\mathcal{H}(q,q') = \langle\Phi(q)|\hat{H}|\Phi(q')\rangle \quad \mathcal{N}(q,q') = \langle\Phi(q)|\Phi(q')\rangle$$

Evaluated with the extended Wick's theorem for overlaps

For the GCM+GOA second derivatives of $\mathcal{H}(q,q')$ are needed

Density dependent interactions

$$V_{DD}(\rho) = t_3 \delta(\vec{r}_1 - \vec{r}_2) \rho^{\alpha}(\frac{1}{2}(\vec{r}_1 + \vec{r}_2))$$

- Phenomenological and very hard (if not impossible) to deduced them from first principles
- They produce a strongly repulsive interaction energy
- State dependent interaction:
  To compute $\langle \Phi | \hat{H}_{DD} | \Phi \rangle$ use $\hat{H}_{DD} = f[\rho]$ with $\rho = \langle \Phi | \hat{\rho} | \Phi \rangle$

how to define the DD interaction for hamiltonian overlaps ?

$$\langle \Phi(q) | \hat{H} | \Phi(q') \rangle$$

Prescriptions

A prescription is required for the calculation of $\langle\Phi(q)|\hat{H}|\Phi(q')\rangle$ in order to compute energies

As it may lead to a complex and/or symmetry breaking density dependent term we have to make sure it yields energies that are

1. real numbers
2. invariant under symmetry transformations (scalar)

we also want to have a framework consistent with the underlying mean field approximation

1. Reduce to the mean field DD term when $|\Phi(q)\rangle = |\Phi(q')\rangle$
2. Produce consistent results for "mean field like" quantities like
   - Chemical potentials
   - RPA equation

Mixed density $\rho_{q,q'} = \langle\Phi(q)|\hat{\rho}|\Phi(q')\rangle / \langle\Phi(q)|\Phi(q')\rangle$

Caveats

- As the mixed density is complex in general and is raised to the power α (1/3 tipically) which Riemman sheet should be choosen for the evaluation of ρ^α ?
- What to do if $\langle\varphi(q)|\varphi(q')\rangle = 0$?
  - This is a rather usual situation in particle number projection as $\langle\varphi|e^{i\phi\hat{N}}|\varphi(q')\rangle = 0$ when $\phi = \pi/2$ and one of the occupancies $v_k^2 = 1/2$. This is part of the famous "pole" problem (M. Anguiano et al Nucl. Phys. A696 (2001) 467)
  - In this case the mixed density diverges !
    But the singularity is integrable if $\alpha < 1$
  - The same kind of singularities appear in "number parity projections"

These questions need to be addressed before we can move forward

and of course Skyrme like or relativistic like interactions have the same problem ...