Nuclear Energy Density Functionals

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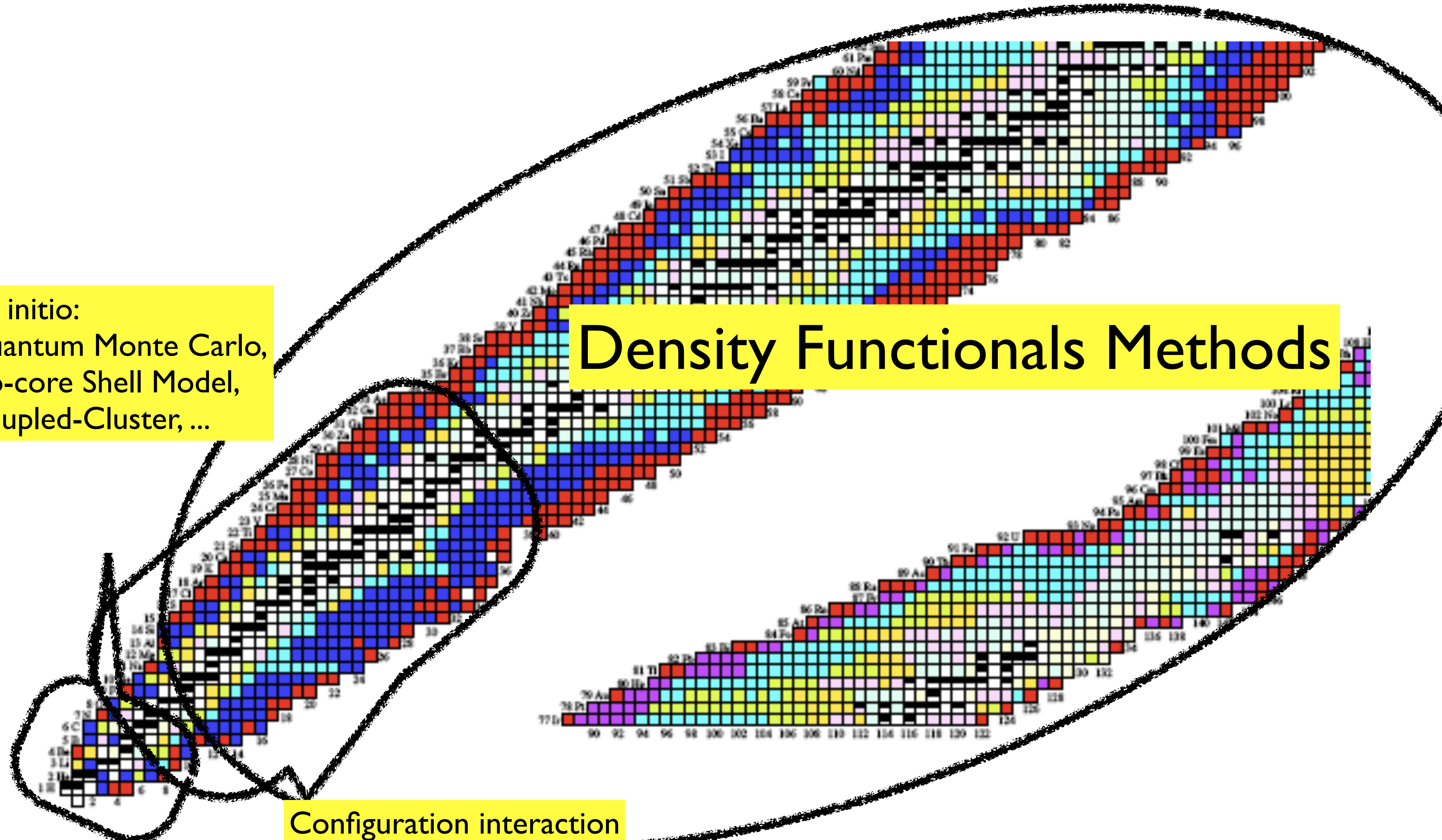
Energy Density Functionals



Nuclear Energy Density Functionals: the many-body problem is mapped onto a one body problem without explicitly involving inter-nucleon interactions!

Self-consistent Kohn-Sham DFT: includes correlations and therefore goes beyond the Hartree-Fock. It has the advantage of being a **local scheme**.

$$v_s[\rho(\mathbf{r})] = v(\mathbf{r}) + U[\rho(\mathbf{r})] + v_{xc}[\rho(\mathbf{r})]$$

external potential | Hartree term | exchange-correlation

$$v_{xc}[\rho(\mathbf{r})] = \frac{\delta E_{xc}[\rho(\mathbf{r})]}{\delta \rho(\mathbf{r})}$$

The practical usefulness of the Kohn-Sham scheme depends entirely on whether accurate approximations for E_{xc} can be found!

... accurate and controlled approximations for the nuclear exchange-correlation energy functional

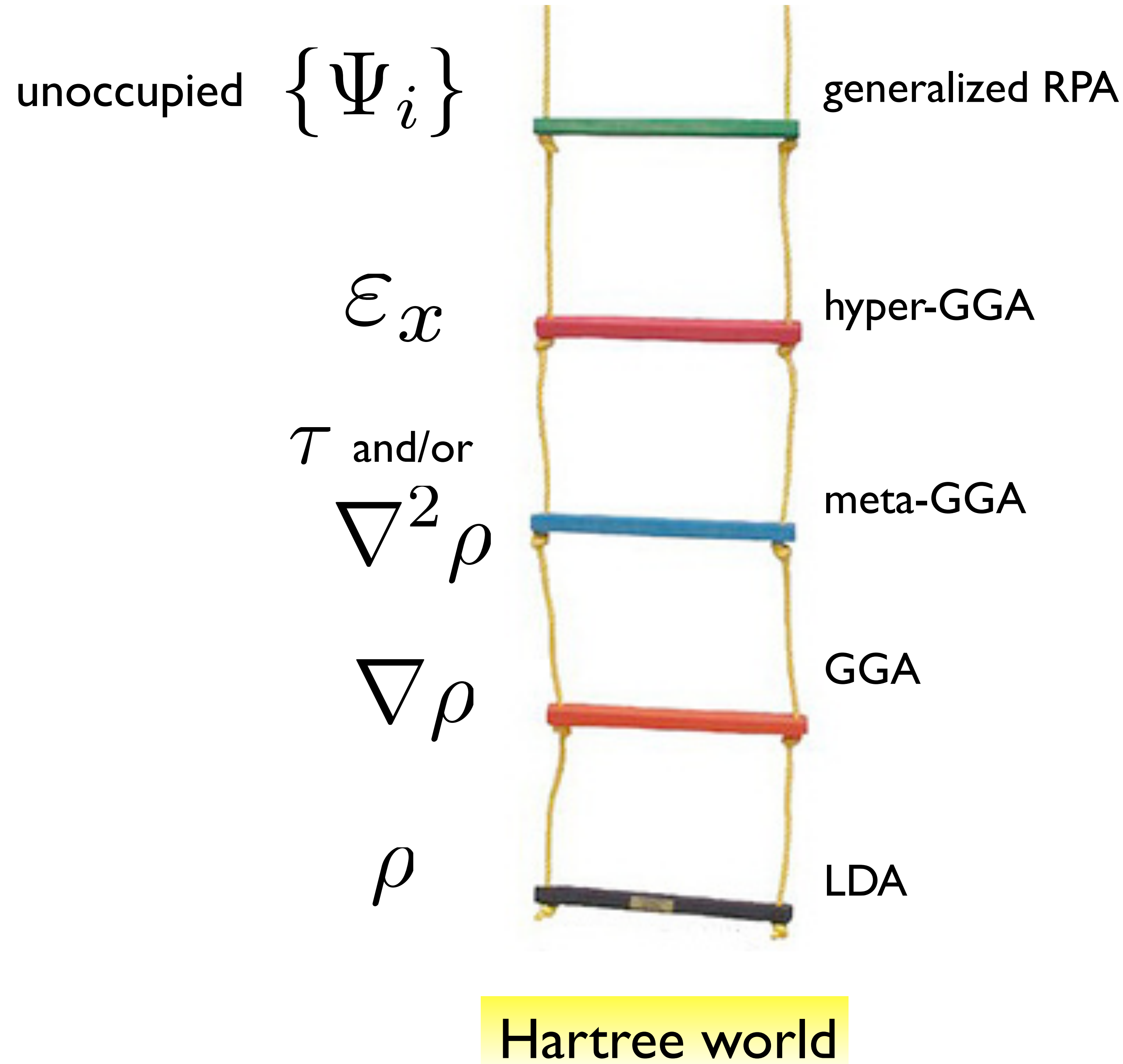
... microscopic foundation for a universal EDF framework, related to and constrained by low-energy QCD

... extensions that include non-nucleonic degrees of freedom

... correlations related to restoration of broken symmetries and fluctuations of collective coordinates

Exchange-correlation functional:

The true E_{xc} is a universal functional of the density: it has the same functional form for all systems.



Jacob's ladder of DFT approximations for E_{xc}

Nuclear Many-Body Correlations

short-range
(hard repulsive core of the NN-interaction)

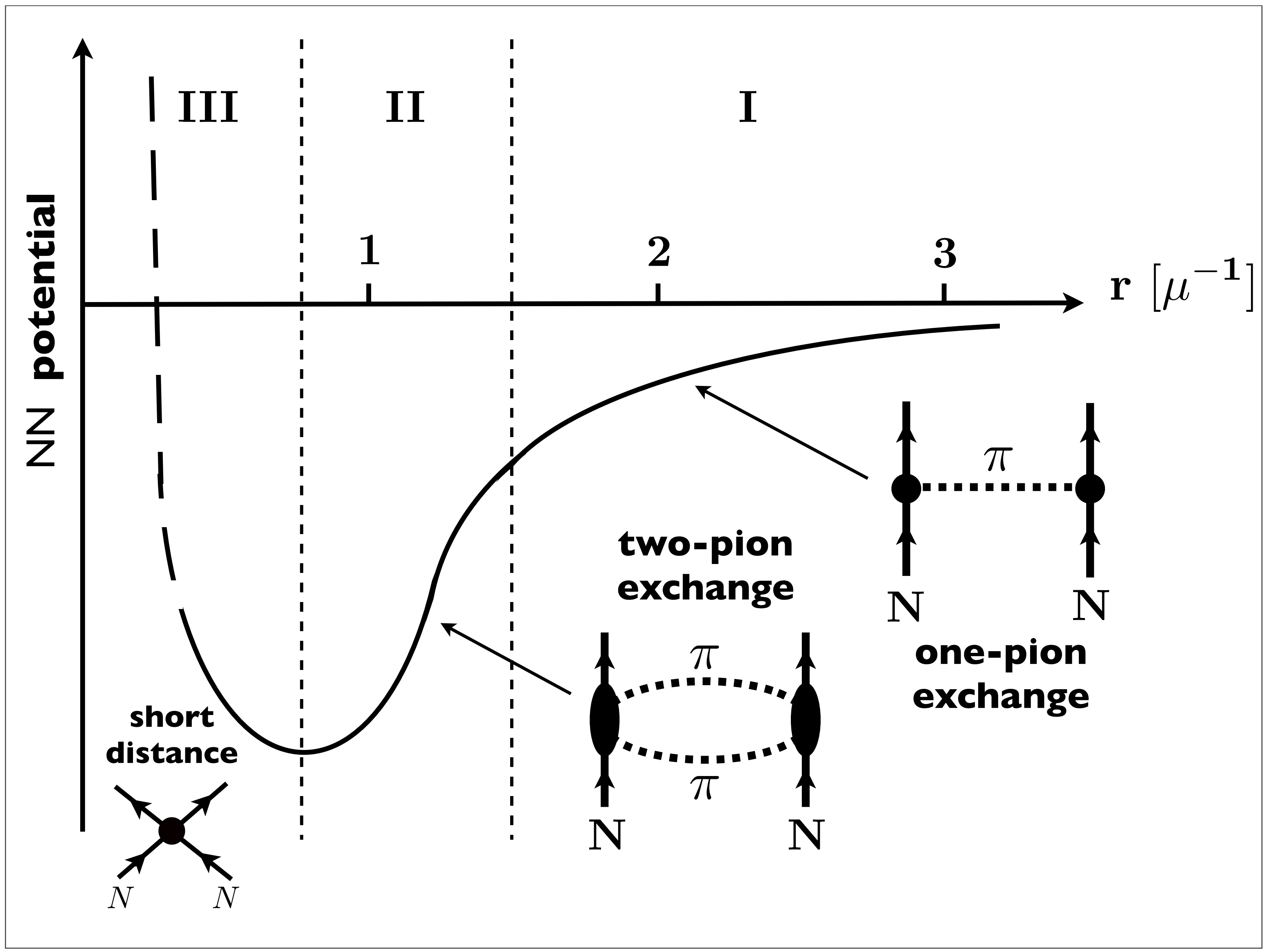
long-range
nuclear resonance modes
(giant resonances)

collective correlations
large-amplitude soft modes:
(center of mass motion, rotation, low-energy quadrupole vibrations)

...vary smoothly with nucleon number!
Can be included implicitly in an effective Energy Density Functional.

A **microscopic nuclear energy density functional** must start from the relevant active degrees of freedom at low energy:

PIONS & NUCLEONS



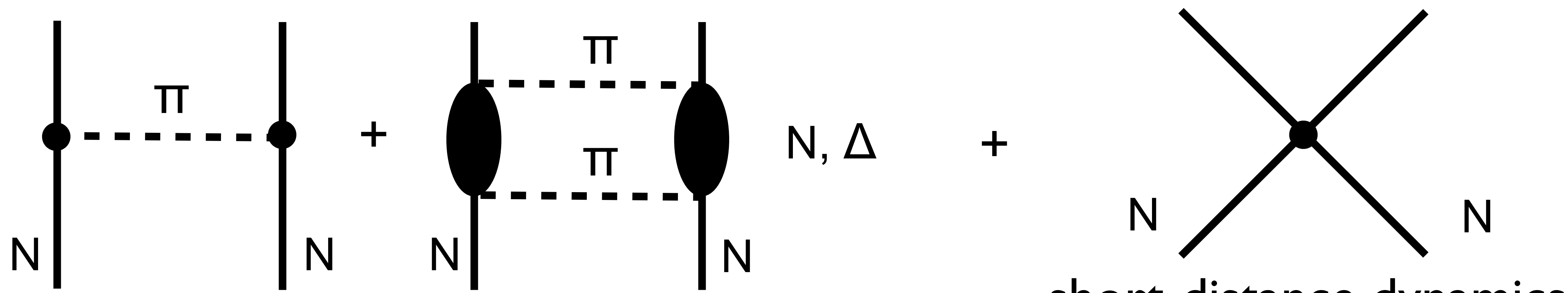
Effective Field Theory of low-energy in-medium NN interactions ⇒ approximations to **the exact exchange-correlation functional.**

In the nuclear medium:

relevant scale:
Fermi momentum

$$k_f \approx 2m_\pi << 4\pi f_\pi$$

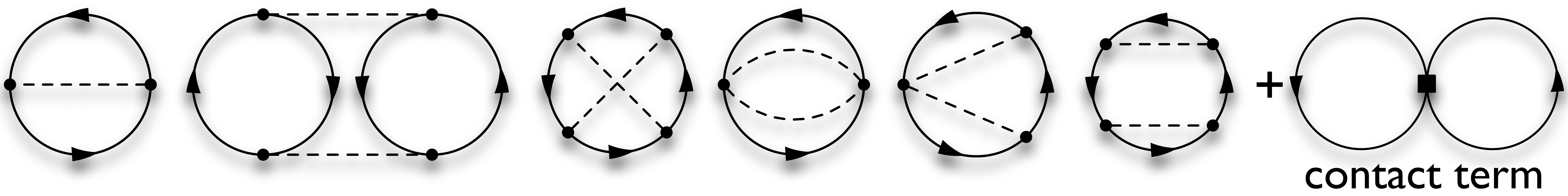
pion-exchange processes in the presence of a filled Fermi sea:



short-distance dynamics

The density functional involves an expansion of nucleon self-energies in **powers of the Fermi momentum.**

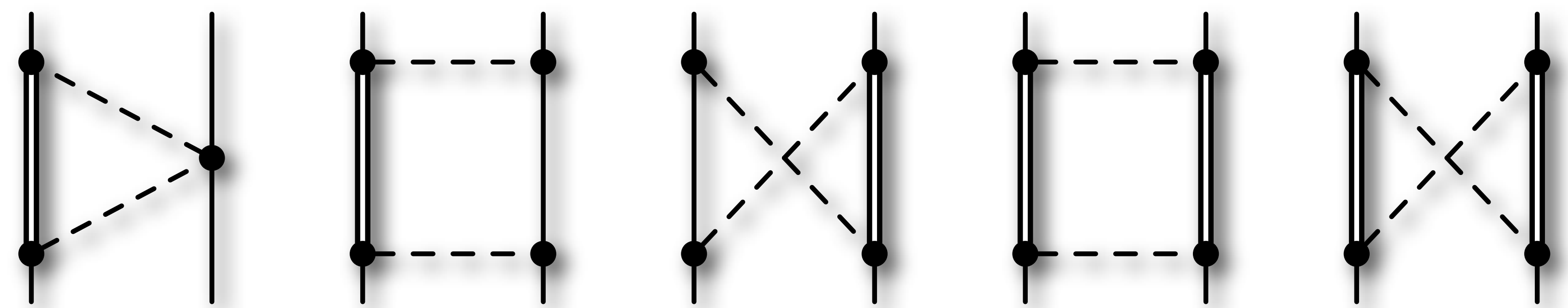
NUCLEAR MATTER Equation of state



$$\overline{E}(k_f) = \frac{3k_f^2}{10\,M_N} - \alpha\left(\frac{k_f}{m_\pi}\right)\frac{k_f^3}{M_N^2} + \beta\left(\frac{k_f}{m_\pi}\right)\frac{k_f^4}{M_N^3} + \cdots$$

Inclusion of the Δ(1232) degree of freedom: $M_\Delta - M_N \approx k_f \approx 2m_\pi$

Two-pion exchange diagrams with single and double Δ(1232) excitations:



Model for Finite Nuclei

P. Finelli, N. Kaiser, D. Vretenar, W. Weise, Nucl. Phys. A **735** (2004) 449, A **770** (2006) 1.

... universal exchange-correlation functional $E_{xc}[\rho]$

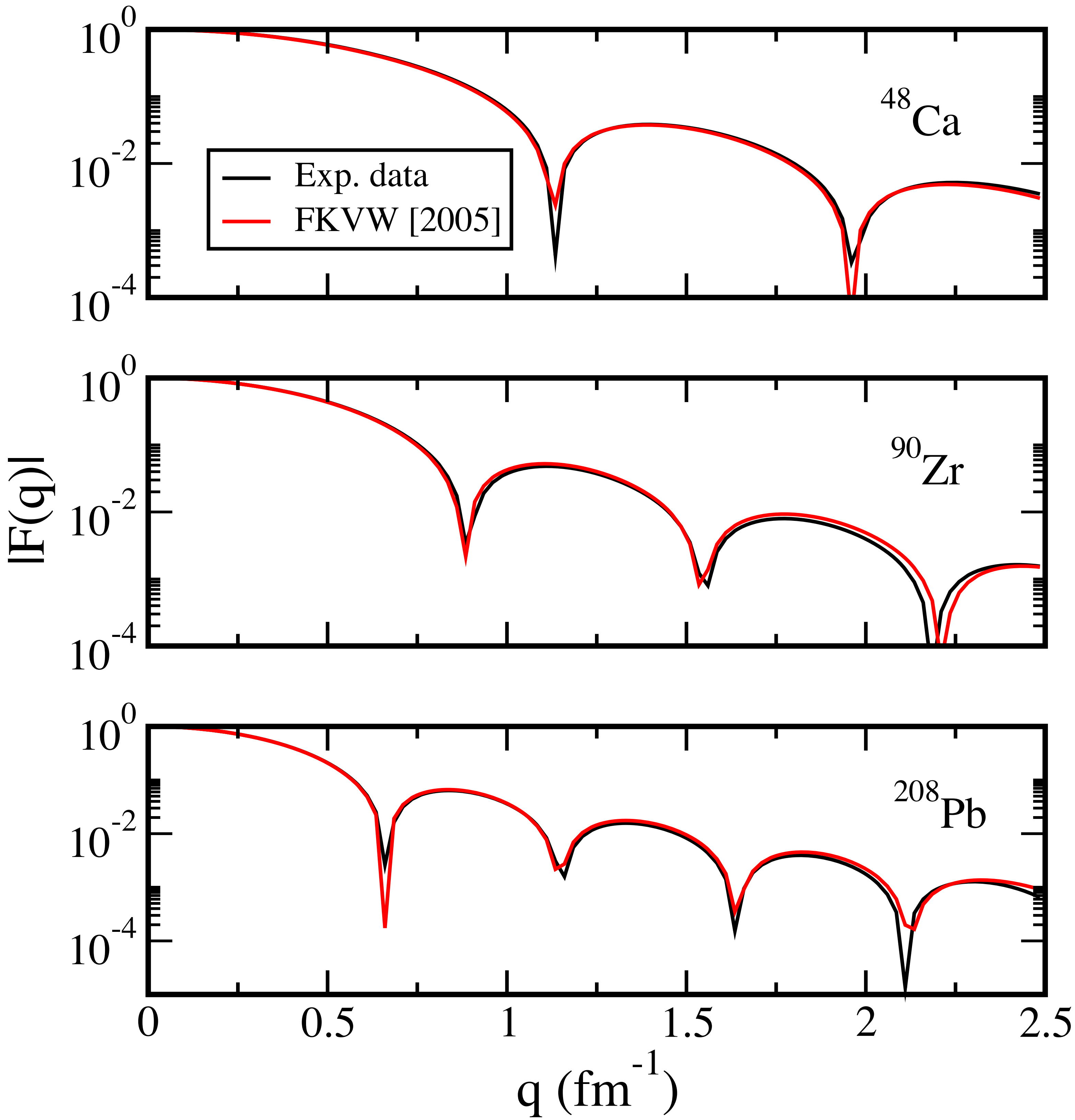
1st step: **Local Density Approximation**

$$E_{xc}^{LDA} \equiv \int \varepsilon^{ChPT}[\rho(\mathbf{r})]\rho(\mathbf{r})d^3r$$

2nd step: **second-order gradient correction to the LDA**

ChPT calculations for inhomogeneous nuclear matter:

$$\mathcal{E}(\rho, \nabla\rho) = \rho\,\overline{E}(k_f) + (\nabla\rho)^2\, F_\nabla(k_f) + \ldots$$



Charge form factors of ^{48}Ca, ^{90}Zr and ^{208}Pb calculated with the FKVW functional, in comparison with the experimental form factors.

CHIRAL EFT provides a consistent microscopic framework for the isoscalar and isovector channels of a **universal nuclear energy density functional**.

Hypernuclear single particle spectra based on in-medium chiral SU(3) dynamics

P. Finelli, N. Kaiser, D. Vretenar, W. Weise, Nucl. Phys. A **831** (2009) 163.

Hypernuclear energy density functional:

$$E[\rho] = E^N[\rho] + E^{\Lambda}_{\rm free}[\rho] + E^{\Lambda}_{\rm int}[\rho]$$

hypernuclear ground state

$$E^{\Lambda}_{\rm free} = \int d^3r \langle \Phi_0 | \bar{\psi}_\Lambda [-i\boldsymbol{\gamma}\cdot\boldsymbol{\nabla} + M_\Lambda] \psi_\Lambda | \Phi_0 \rangle$$

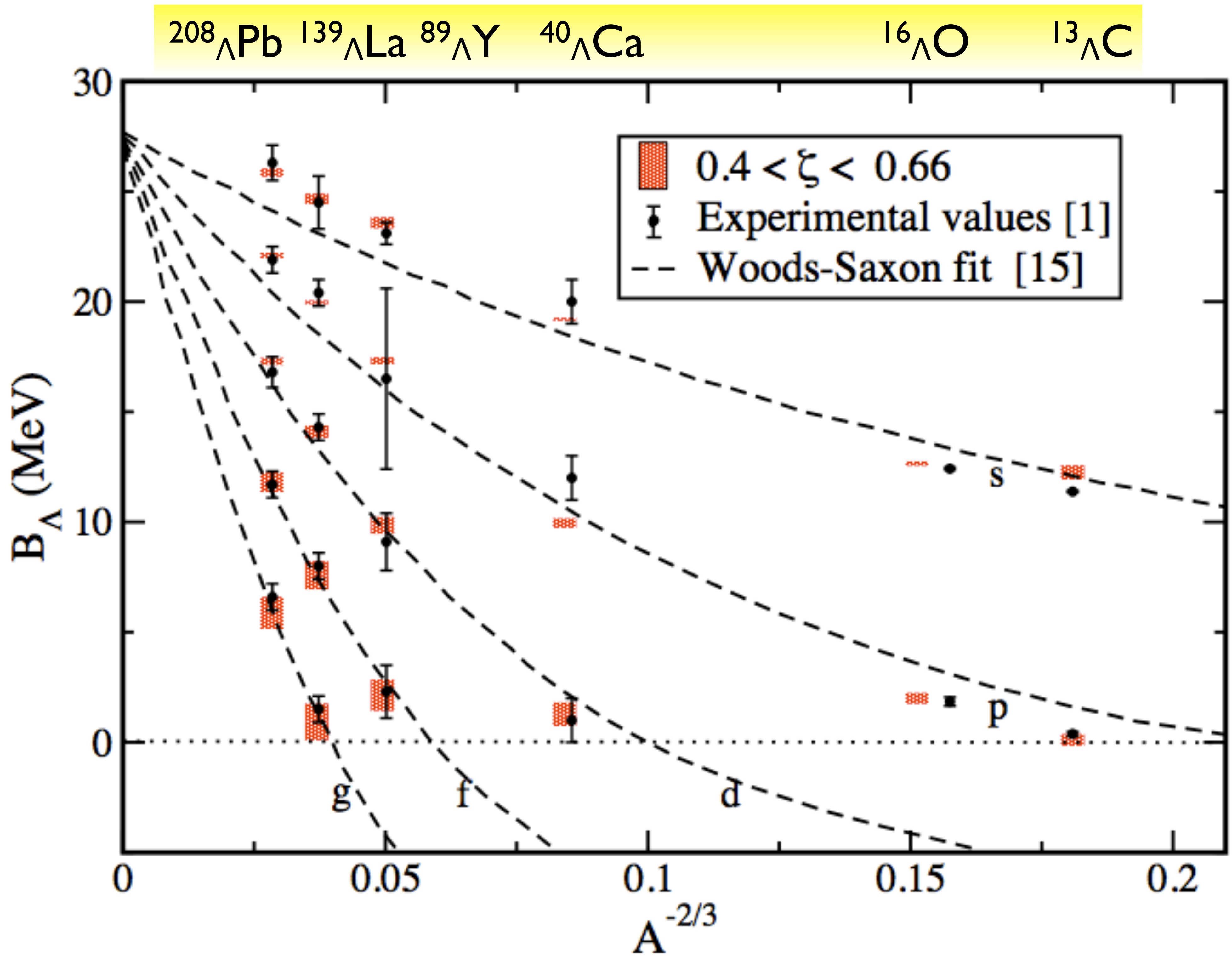
coupling to the scalar nucleon density

$$E^{\Lambda}_{\rm int} = \int d^3r \, \{ \langle \Phi_0 | G^{\Lambda}_S(\rho) \, (\bar{\psi}\psi) \, (\bar{\psi}_\Lambda \psi_\Lambda) \, | \Phi_0 \rangle + \langle \Phi_0 | G^{\Lambda}_V(\rho) \, (\bar{\psi}\gamma_\mu\psi) \, (\bar{\psi}_\Lambda \gamma^\mu \psi_\Lambda) \, | \Phi_0 \rangle + \langle \Phi_0 | D^{\Lambda}_S \, \partial_\mu(\bar{\psi}\psi) \, \partial^\mu(\bar{\psi}_\Lambda \psi_\Lambda) | \Phi_0 \rangle \}$$

coupling to the vector nucleon density

derivative term - from a gradient expansion of the EDF

Binding energies of the Λ in different s, p,... orbitals of six hypernuclei:



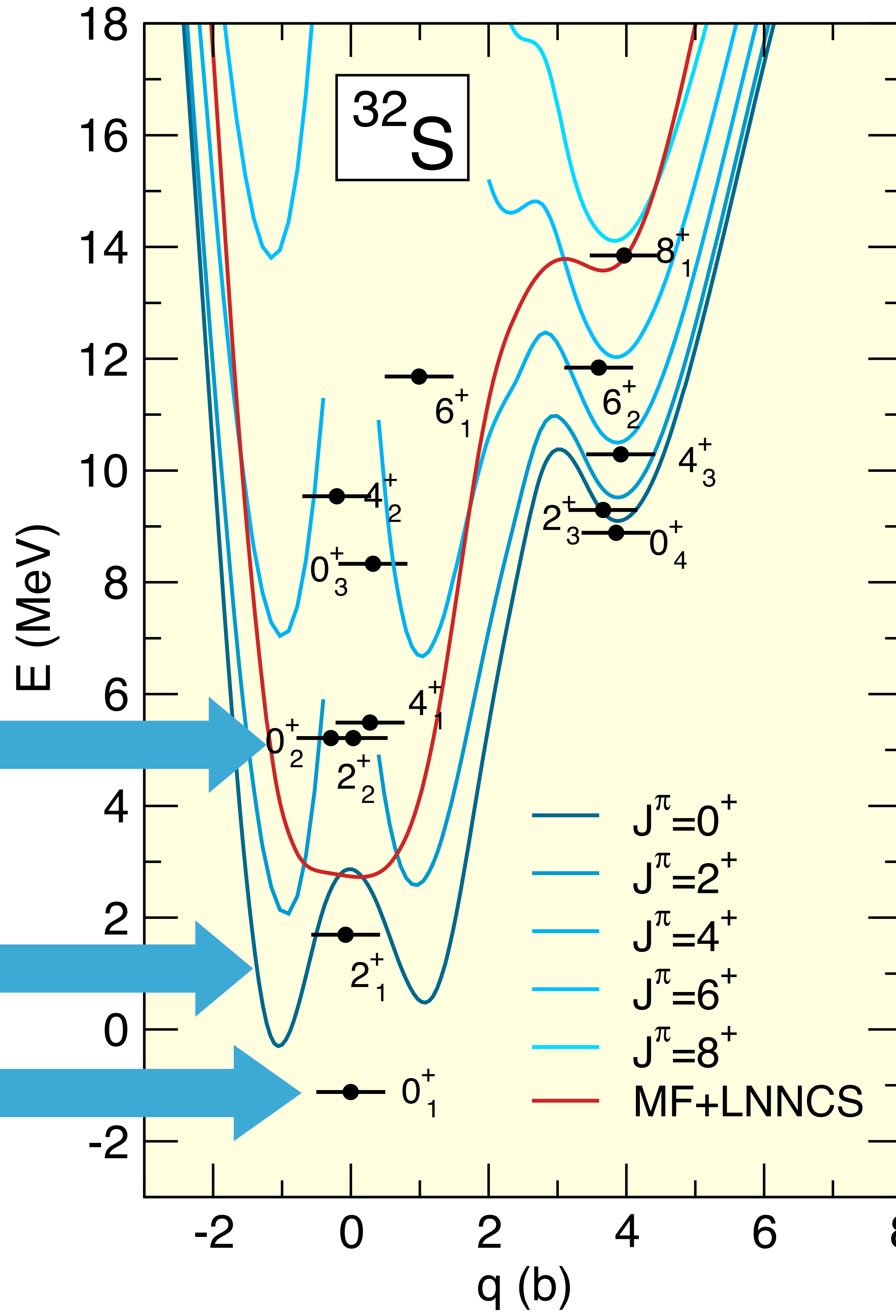
Collective correlations: restoration of broken symmetries and fluctuations of collective variables

Nikšić, Vretenar, Ring
Phys. Rev. C **73**, 034308 (2006)
Phys. Rev. C **74**, 064309 (2006)

1. Mean-field calculations, with a constraint on the quadrupole moment.

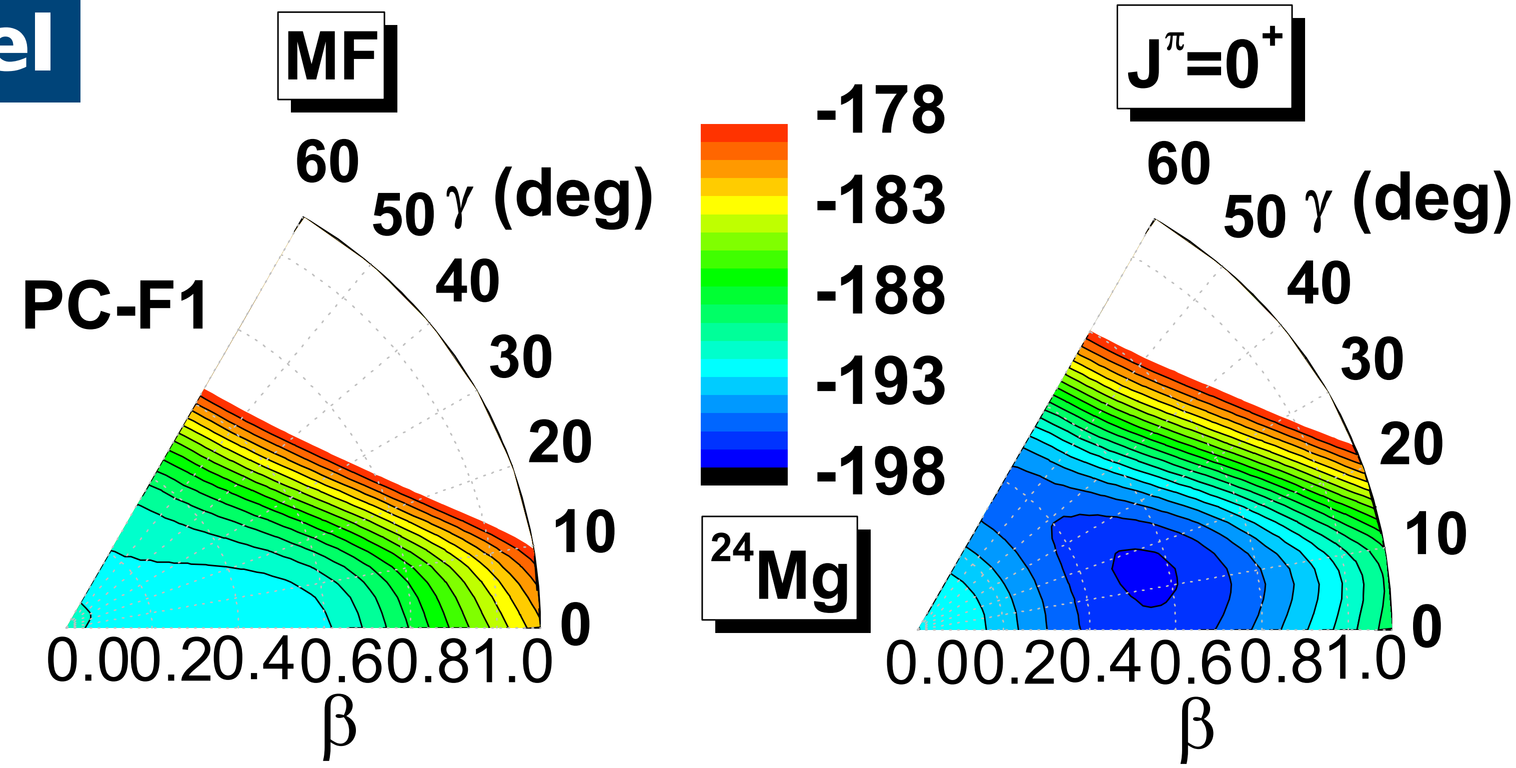
2. Angular-momentum and particle-number projection.

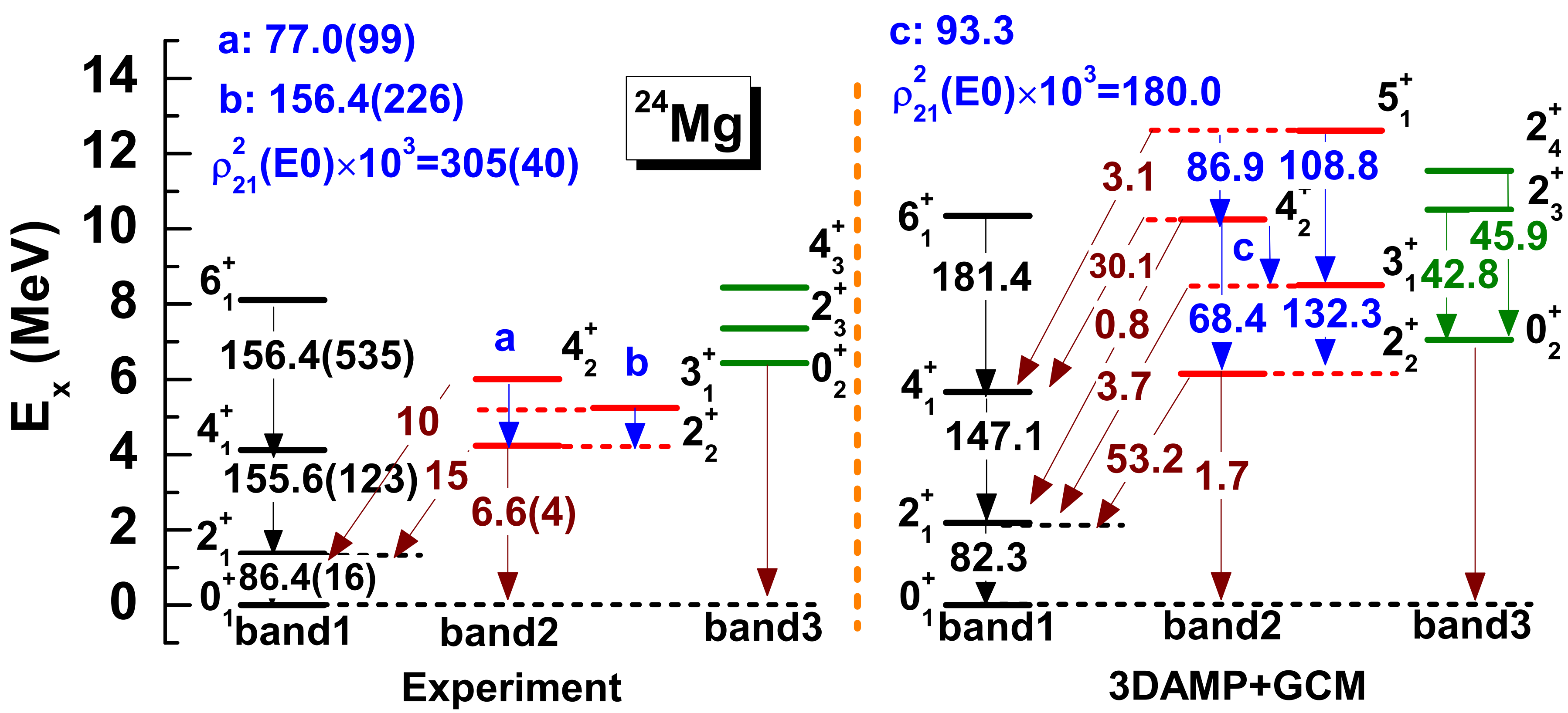
3. Generator Coordinate Method ⇒ configuration mixing



... larger variational space for projected GCM calculations!

3D AMP + GCM model





Yao, Meng, Ring, Vretenar,
Phys. Rev. C **81**, 044311 (2010)

Five-dimensional collective Hamiltonian

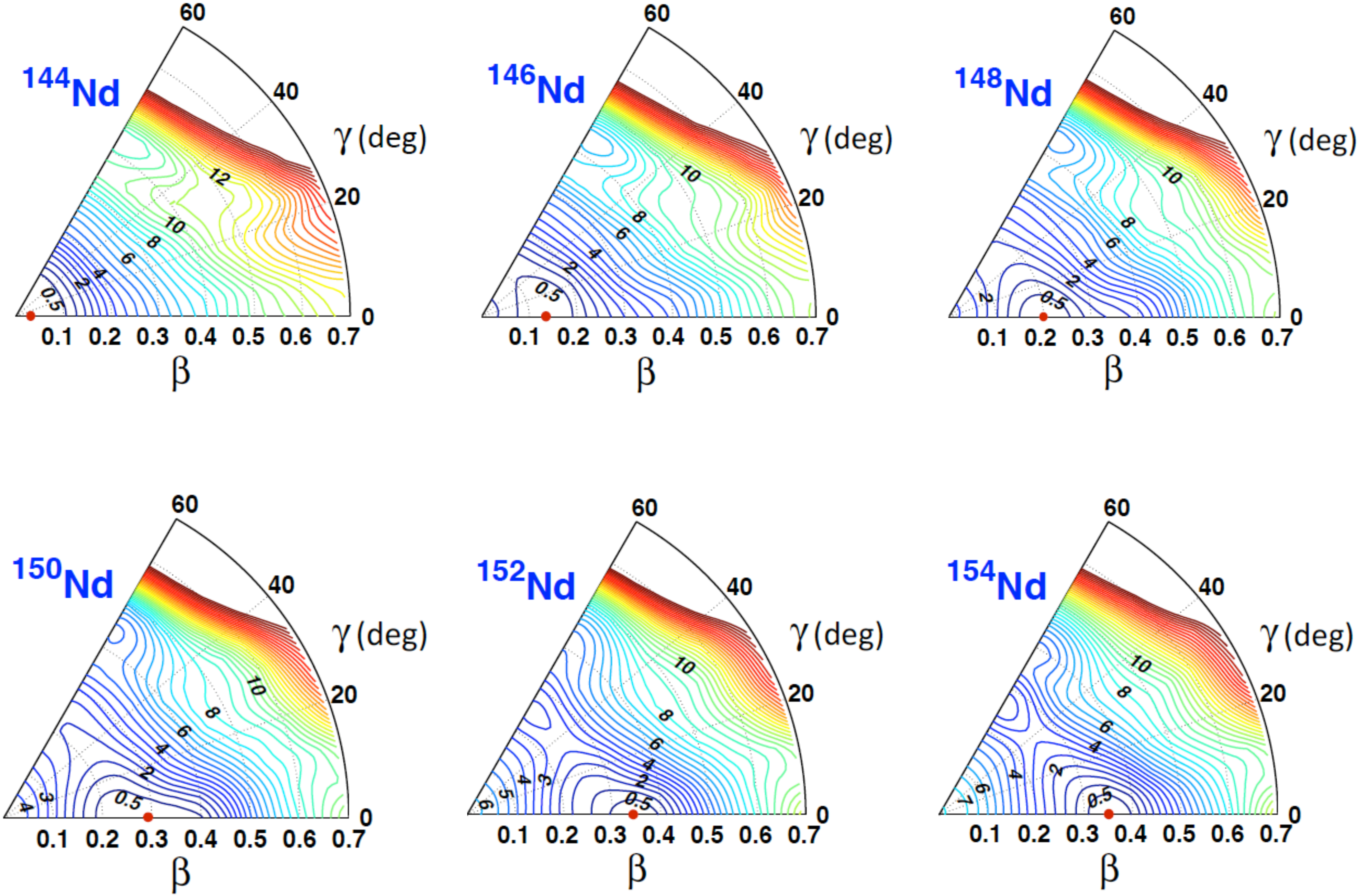
Nikšić, Li, Vretenar, Prochniak, Meng, Ring, Phys. Rev. C **79**, 034303 (2009)

... nuclear excitations determined by quadrupole vibrational and rotational degrees of freedom

$$H_{\text{coll}} = \mathcal{T}_{\text{vib}}(\beta,\gamma) + \mathcal{T}_{\text{rot}}(\beta,\gamma,\Omega) + \mathcal{V}_{\text{coll}}(\beta,\gamma)$$

$$\mathcal{T}_{\text{vib}} = \frac{1}{2}B_{\beta\beta}\dot{\beta}^2 + \beta B_{\beta\gamma}\dot{\beta}\dot{\gamma} + \frac{1}{2}\beta^2 B_{\gamma\gamma}\dot{\gamma}^2$$

$$\mathcal{T}_{\text{rot}} = \frac{1}{2}\sum_{k=1}^{3}\mathcal{I}_k\omega_k^2$$



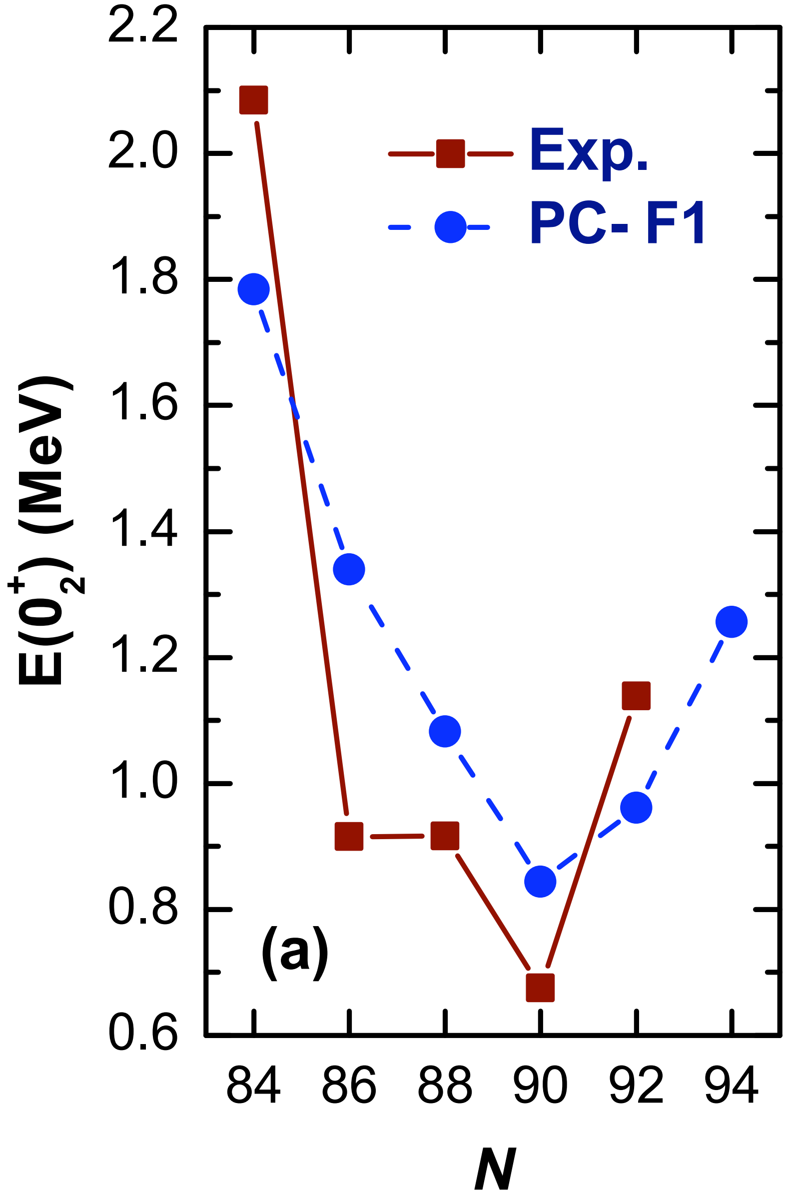
Li, Nikšić, Vretenar, Meng, Lalazissis, Ring, Phys. Rev. C **79**, 054301 (2009)

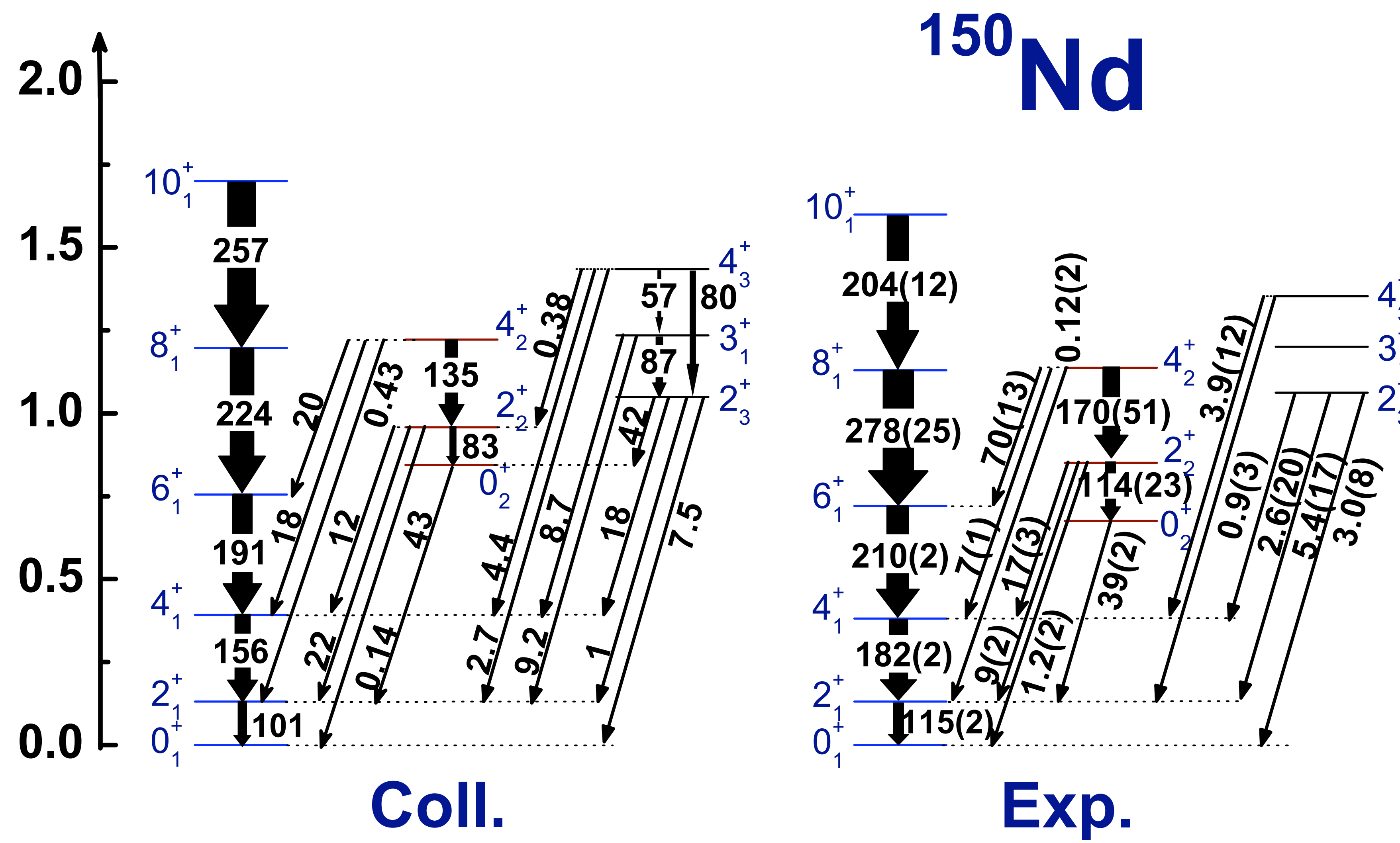
EDF description of nuclear Quantum Phase Transitions

Nikšić, Vretenar, Lalazissis, Ring, Phys. Rev. Lett. **99**, 092502 (2007)

Li, Nikšić, Vretenar, Meng, Lalazissis, Ring, Phys. Rev. C **79**, 054301 (2009)

Order parameter





... detailed spectroscopy in the EDF framework!

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