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# Energy Density Functional Methods

## Modern view and undergoing developments

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# Outline

1. EDF methods

- Basic features
- Current focuses

2. Gamma ray spectroscopy

- Natural interplay; e.g. shell evolution, transact., shape coex.
- Example: shape coexistence in neutron deficient Kr isotopes

3. Making EDF methods more predictive and reliable

- Constructing *non-empirical* energy functionals
- Regularizing *spurious* contributions to MR calculations

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# 1. EDF methods

## Basic features

## Current focuses

# Energy Density Functional methods: basics

## Basic elements

- Approaches not based on a correlated wave-function
- Energy is postulated to be a functional of one-body density (matrices) $\mathcal{E}[\rho, \kappa, \kappa^*]$
- Symmetry breaking is at the heart of the method
- Two formulations (i) Single-Reference (ii) Multi-Reference

## Pros

- Use of full single-particle space
- Collective picture but fully quantal
- Universality of the EDF ($A \gtrsim 16$)
- Ground state description
- Static (smooth) correlations

## Cons

- No universal parametrization
- Empirical = limited predictive power
- Spectroscopy / odd nuclei
- Dynamical (fluctuating) correlations
- Limited accuracy ($\sigma_{rms}^{mass} \approx 700$ keV)

### Single-Reference « Mean-field »

- *Nuclear equation of state*
- *Binding and separation energies*
- *Shell structure and pairing gaps*
- *Fission and deformation properties*
- *Charge densities, neutron skin, radii*
- *Individual and rotational excitations*
- *Halos*

### Multi-Reference « Beyond mean-field »

- *All what is calculated in SR*
- *Dynamical correlations in the g.s.*
- *Vibrational excitations*
- *LACM and shape coexistence*
- *E.M. transitions in the lab frame*

- Skyrme = **quasi-local** / Gogny = **non-local**
- Parameters adjusted on a set of data (bias on bulk properties so far)
- Similar good performances for properties of known nuclei
- "Asymptotic freedom" as one jumps into the ***next major shell***

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# Present focuses

- **Spectroscopy**
  - Shell evolution
    - 1qp states in odd nuclei -> Shape/spin polarization, purity of states
    - 1qp states, K-isomers and rotational states in transactinides
    - Enriched EDF ->Tensor, spin orbit, density dependencies
  - Spectroscopy of collective modes
    - Complex nuclei -> Triaxiality, cranking
    - First $2^+$ in semi-magic nuclei -> Triaxiality, coupling to 2qp states

- **Predictive power**
  - Improved fitting protocole
    - Better use of existing/new data -> superdef, odd, neutron rich
    - Fitting algorithm and post analysis methods
  - Construct *non-empirical* energy functional from NN/NNN

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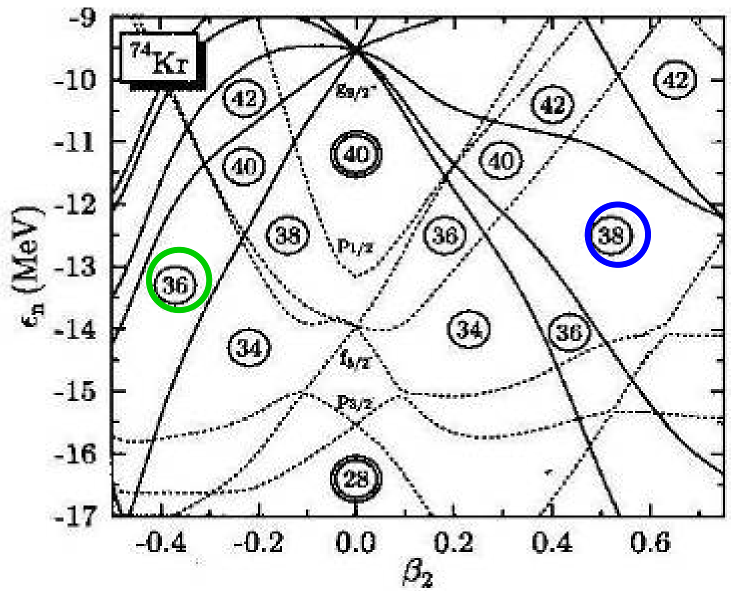
## 2. Gamma ray spectroscopy

### Shape coexistence in neutron-deficient Kr isotopes

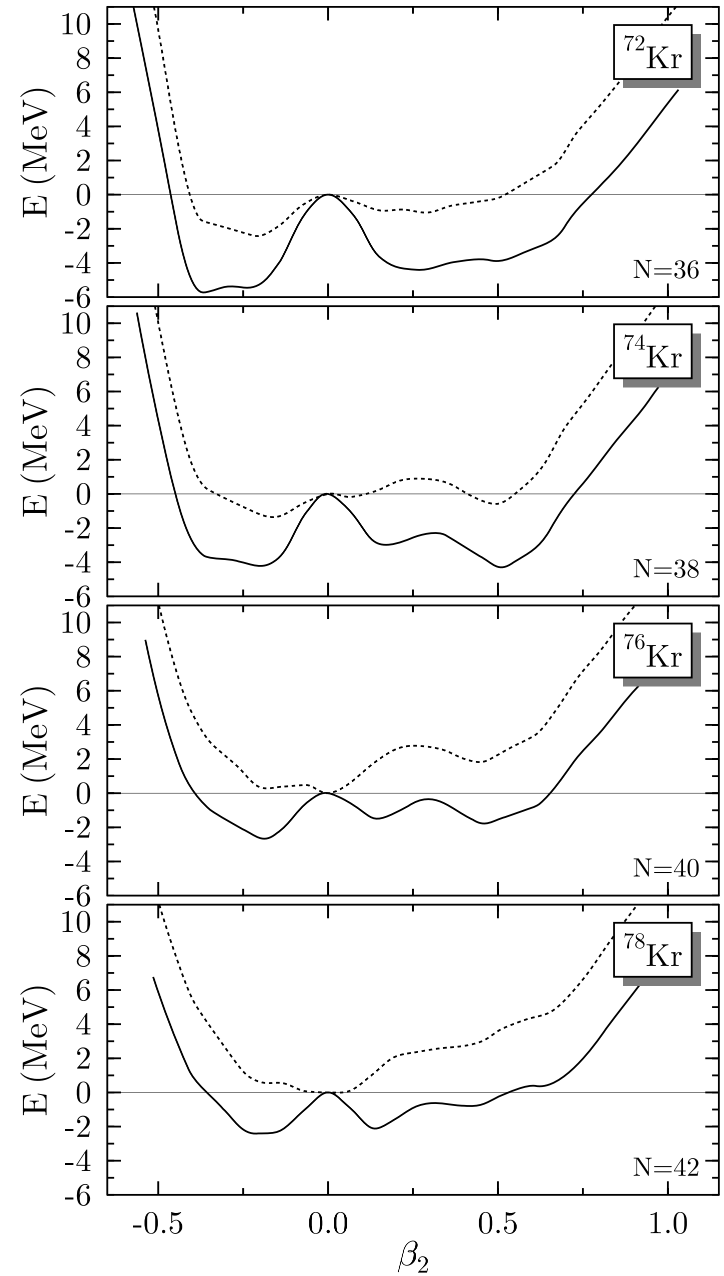
# Shape coexistence in light Kr isotopes



M. Bender et al., PRC 74, 024312 (2006)



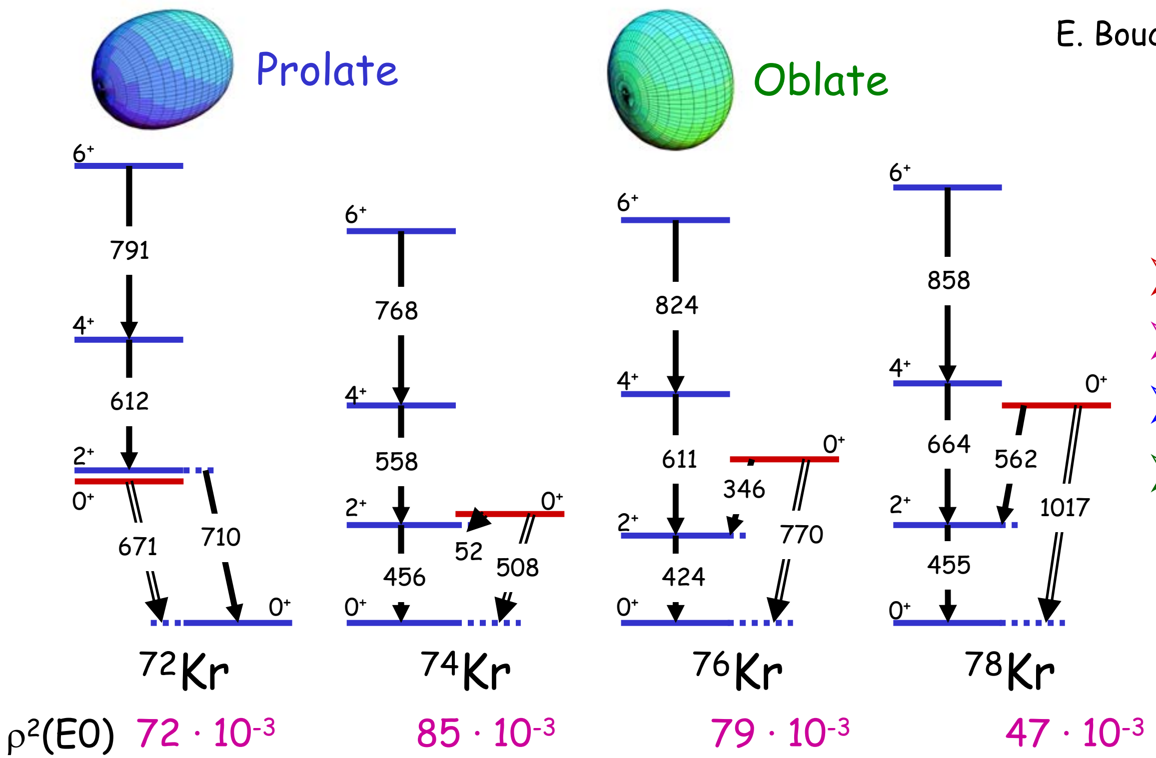

Oblate Prolate




- Several obl./prol./spher. gaps at 36, 38, 40
- Shape coexistence expected in Kr, Se…
- Confirmed by SR calculation (Skyrme)
  - **Oblate shape favored from $^{72}$Kr to $^{78}$Kr**
- Proj. on J (MR calc.) brings prolate minima down

# Systematics of the light krypton isotopes

E. Bouchez et. al., PRL90 (2003) 082502



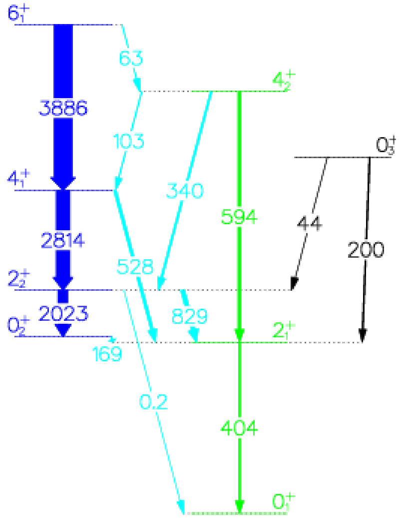

- energy of excited $0^+$
- E0 strengths $\rho^2$(E0)
- configuration mixing
- Inversion of ground state shape for $^{72}$Kr

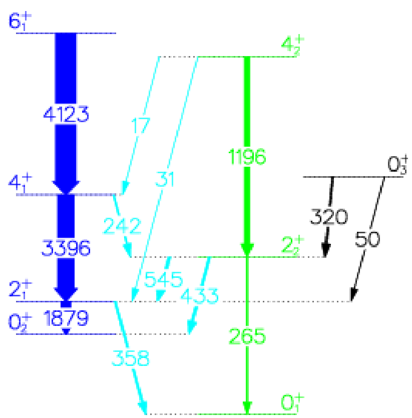
- Exp: determine sign of spectroscopic quadrupole moments Qs directly
  - Low-energy Coulomb excitation of $^{74}$Kr and $^{76}$Kr at SPIRAL
  - Multi-step excitation possible + differential measurement: $d\sigma/d\theta$

- Theory: impact of shape fluctuations and shape mixing through MR calc.?
  - GCM calculation along $Q_{20}$ degrees of freedom (Skyrme)
  - Bohr halmitonian calc. along $Q_{20}$ and $Q_{22}$ degrees of freedom (Gogny)

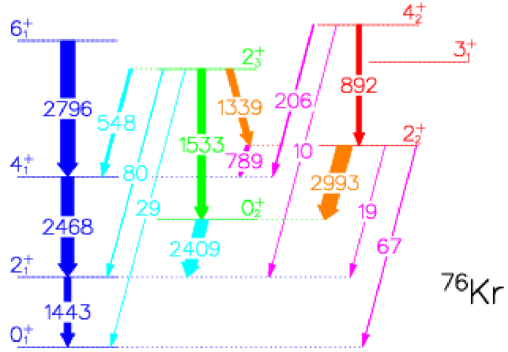
# Comparison between MR calculations and experiment

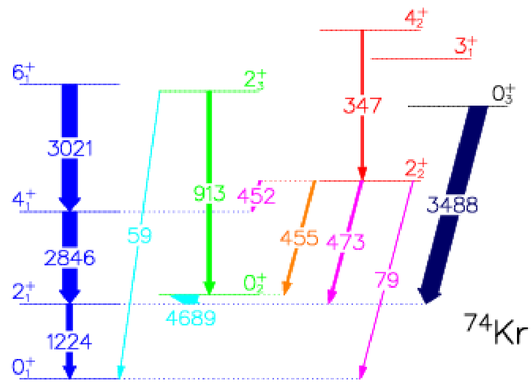
prolate oblate




$Q_s<0$ prolate $Q_s>0$ oblate




GCM calculation
Axial deformation
Skyrme SLy6

M. Bender et al.
PRC 74, 024312 (2006)

Experimental B(E2;↓) [$e^2fm^4$]

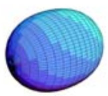
E. Clément et al.,
PRC 75, 054313 (2007)

GCM (GOA) calculation
Triaxial deformation
Gogny D1S

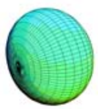
M. Girod et al., to be published

# Shape transition in the light krypton isotopes

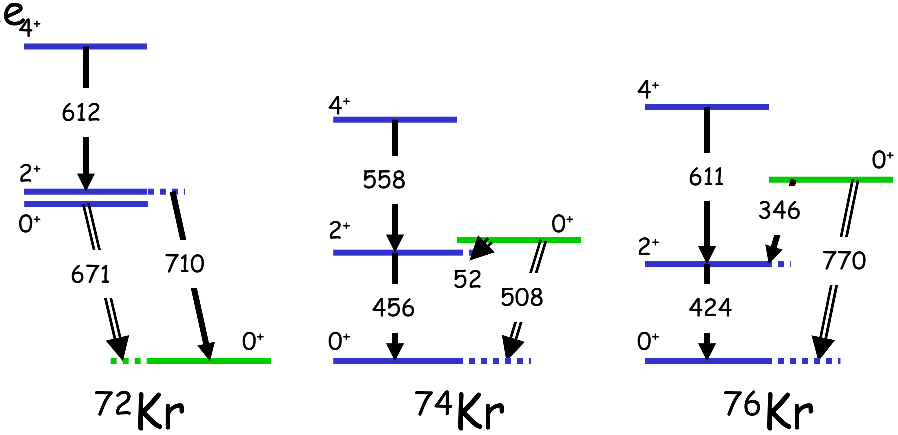
- Direct and indirect experimental evidence



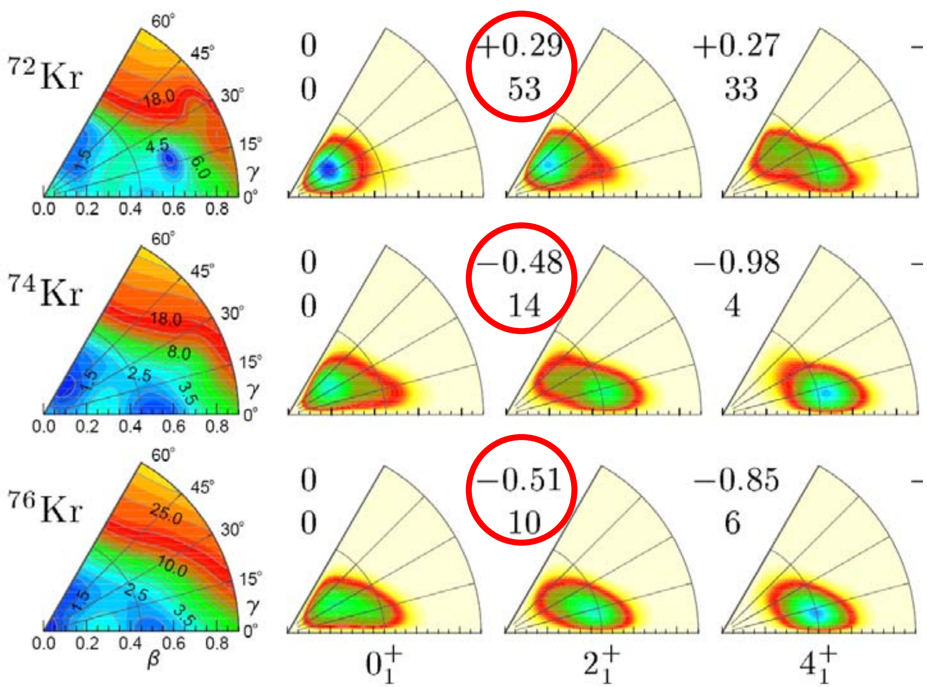
Prolate



Oblate



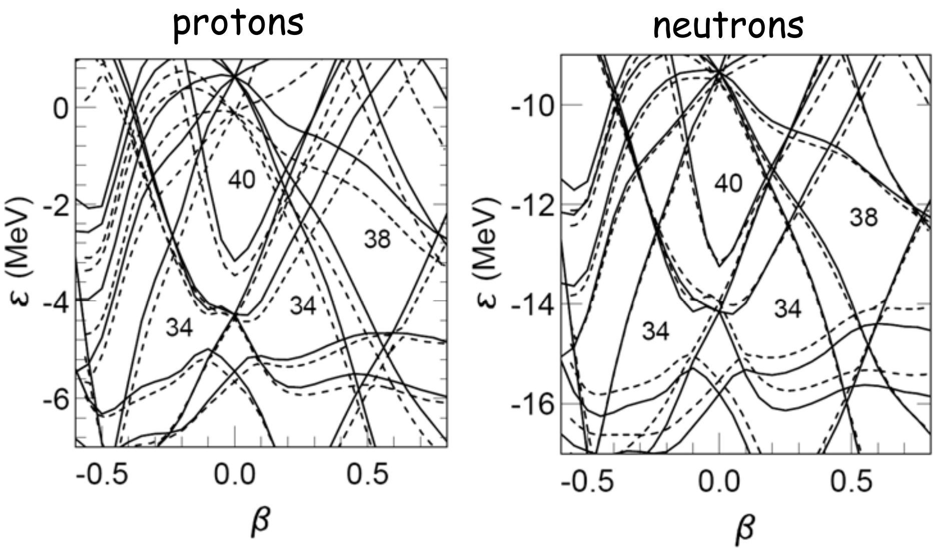

- Collective wave-function from Gogny D1S 5D Bohr-Hamiltonian calculation




- Clear shape transition through 74Kr
- **Mixing of triaxial shapes is essential**
- Mixing of K=0 and K=2 states

M. Girod et al., to be published

# Comparison of Multi-Reference configuration mixing calculations




**Difference #1: energy functional**

**Skyrme SLy6** ⇔ **Gogny D1S**
Bender et al. Girod et al.

**Similar s.p. energies on the SR level**

**Difference #2: generator coordinates**

***axial quadrupole deformation*** $q_0$ ⇔ ***triaxial quadrupole deformation*** $q_0$, $q_2$

- Good agreement for in-band B(E2) and quadrupole moments
- Wrong ordering of states: oblate ground-state shape for $^{72}$Kr → $^{78}$Kr
- Excited states dilated in energy
- K=2 states outside model-space

- Excellent agreement for excitation energies, B(E2), and quadrupole moments
- Inversion of ground-state shape from prolate in $^{76}$Kr to oblate in $^{72}$Kr reproduced
- Assignment of prolate, oblate, and K=2 states

1. **Triaxiality is key to describe prolate-oblate shape coexistence in Kr region**
2. **The deficiencies of s.p. spectra pointed out by Bender et al remain**

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## 3. Making EDF methods more predictive and reliable

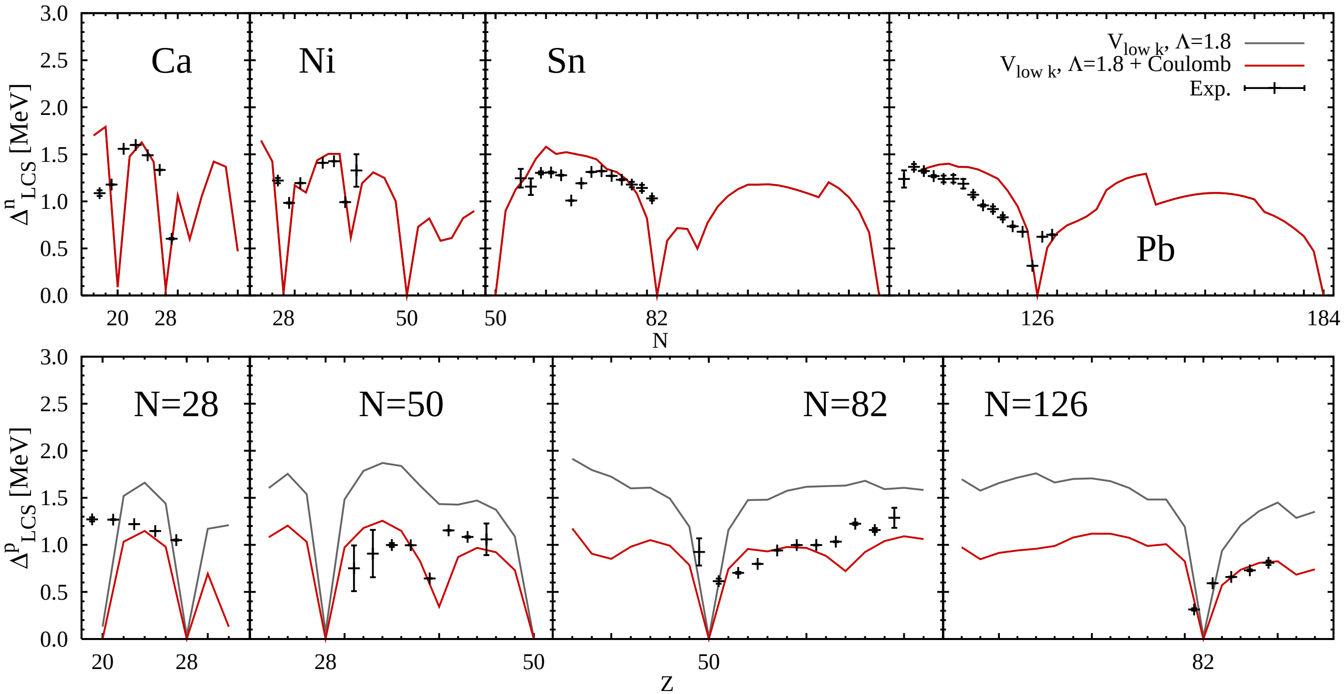
Constructing *non-empirical* energy functionals

Regularizing *spurious* contributions to MR calculations

# Construction of non-empirical (pairing) energy functional

T. Lesinski, T. D., K. Bennaceur, J. Meyer, to be published

- Empirical functionals lack predictive power
- Microscopic origin of nn/pp superfluidity in nuclei?
- Functional constructed at lowest order in bare NN




- Neutron/proton gaps are consistently close to experiment
- Coulomb responsible for 30% decrease of the gaps
- Higher-orders and NNN effects negligeable or cancel out?

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# Removing spurious contributions from MR calculations

- Unexpected spurious content of Particle Number Restoration calculations

J. Dobaczewski, M. V. Stoitsov, W. Nazarewicz, and P.-G. Reinhard PRC76 (2007) 054315

- Regularization method
  - Valid for any MR calculation
  - For integer powers of the density
- Ex: calculation of $^{18}$O with SLy4

D. Lacroix, T. D., M. Bender, to be published

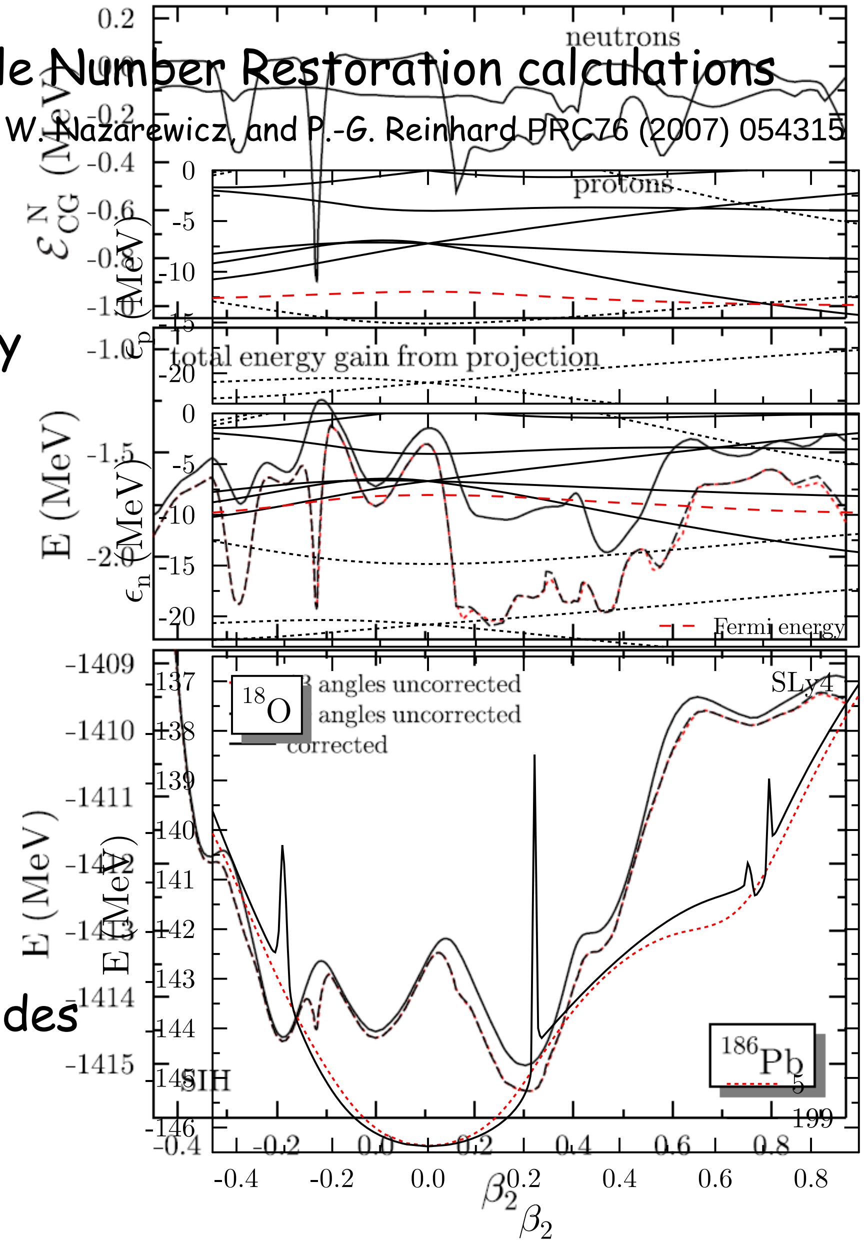
  - Enough integration points
  - Finite spurious steps
- Ex: calculation of $^{186}$Pb with SIII
  - Remove spuriosities
  - Spurious infinities

M. Bender, T. D., D. Lacroix, to be published

  - Modifies topology of PES
  - Same scale as excitations

M. Bender, T. D., D. Lacroix, to be published

- Conclusions
  - Need to implement in all MR codes
  - Need to design new EDFs



# Conclusions and Perspectives

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- EDF methods are becoming a spectroscopic-quality tool

- Lot has been done but lot to do!

  1. Formal issues
  2. Performances of empirical EDFs
  3. Connection to underlying NN/NNN interactions
  4. Extension of existing codes, in particular for MR calculations
  5. Systematic applications to nuclei with extreme N/Z
  6. More applications to systems of experimental interest

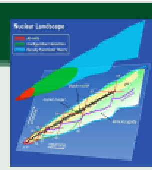
- Perspectives with coming generation of RIB facilities look really good

- More and more interactions with experimentalists expected…

# Ultimate goals

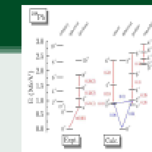
**Ground state**

Mass, deformation



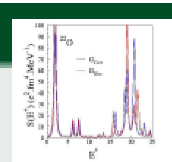
**Spectroscopy**

Spectroscopy



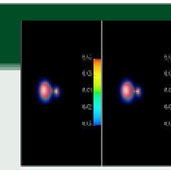
**Collective modes**

RPA, QRPA, GCM



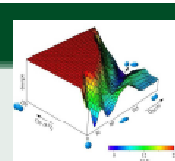
**Reaction properties**

Fusion, transfer, elastic



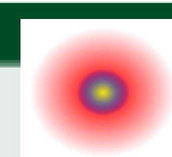
**Heavy elements**

Fission, fusion, SHE



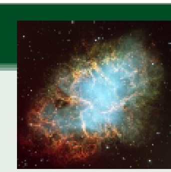
**Exotic behaviors**

Drip-lines, halos



**Astrophysics**

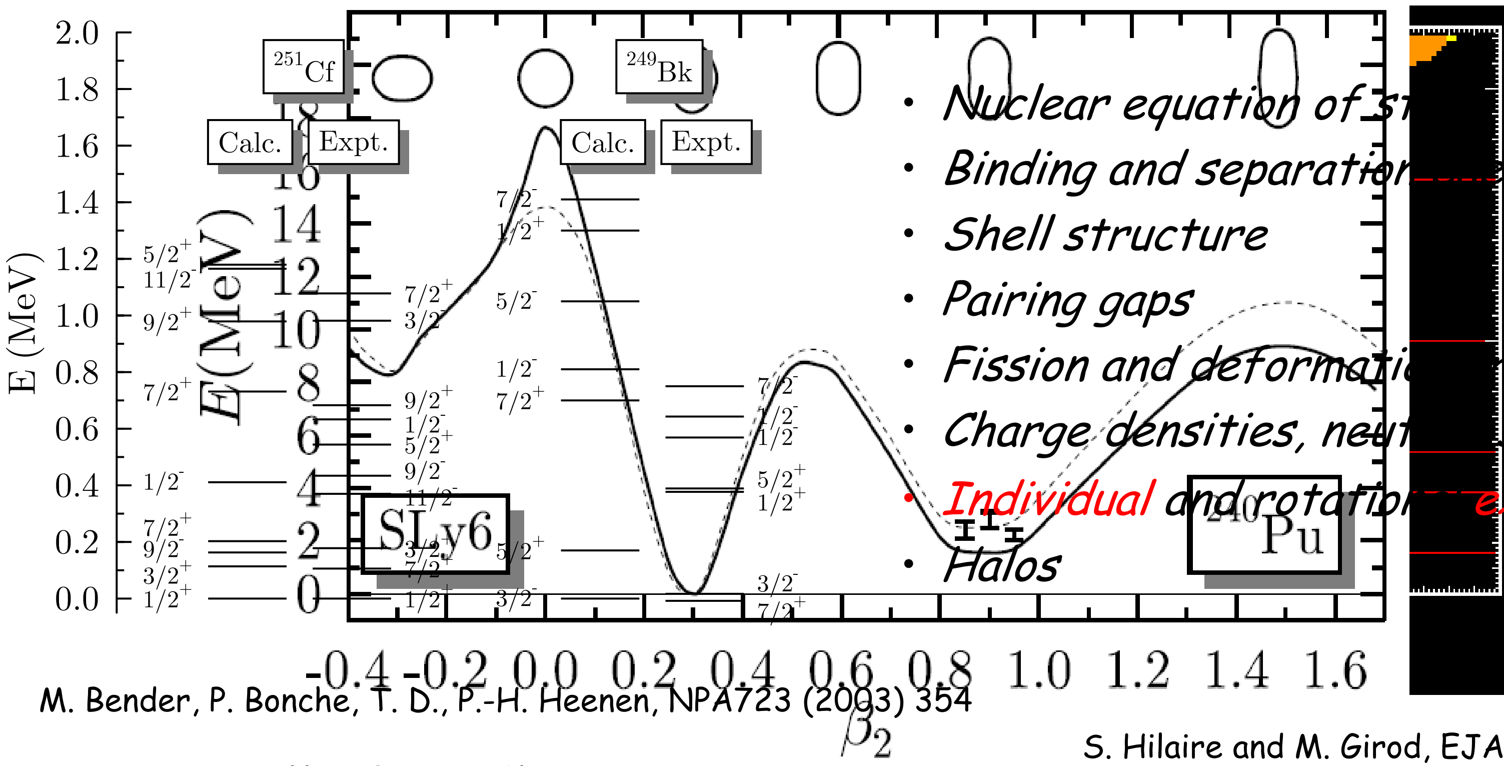
r-process, NS, SN



From underlying NN and NNN interactions

# Single-Reference = « mean-field »

- First level of implementations
- Density matrices ρ and κ constructed from *one* product state
- Incorporates (static) correlations beyond Hartree-Fock




M. Bender, P. Bonche, T. D., P.-H. Heenen, NPA723 (2003) 354

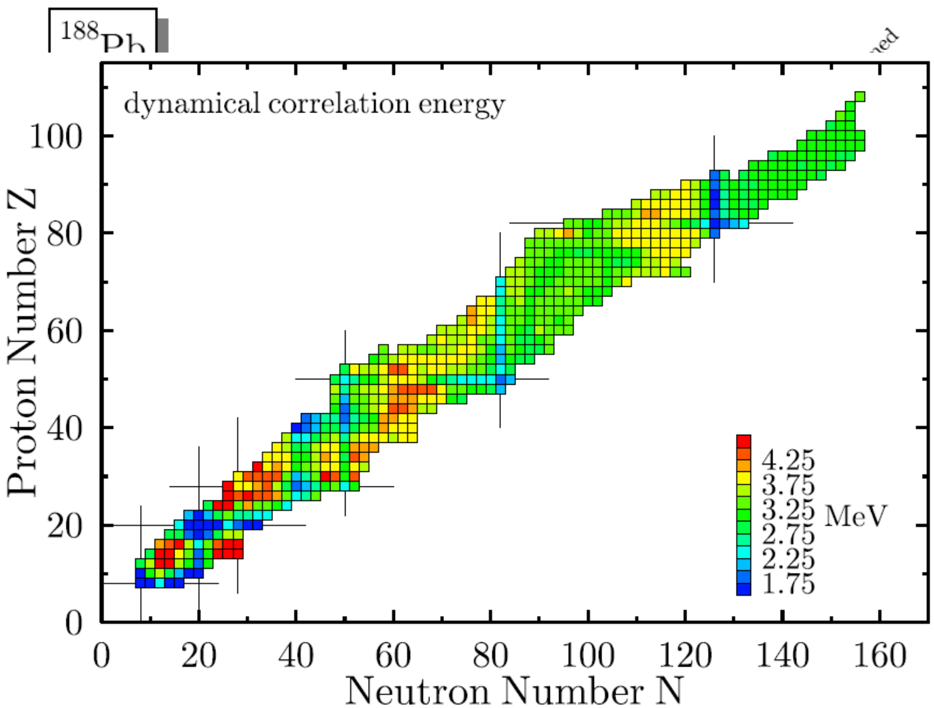
S. Hilaire and M. Girod, EJA 33 (2007) 237

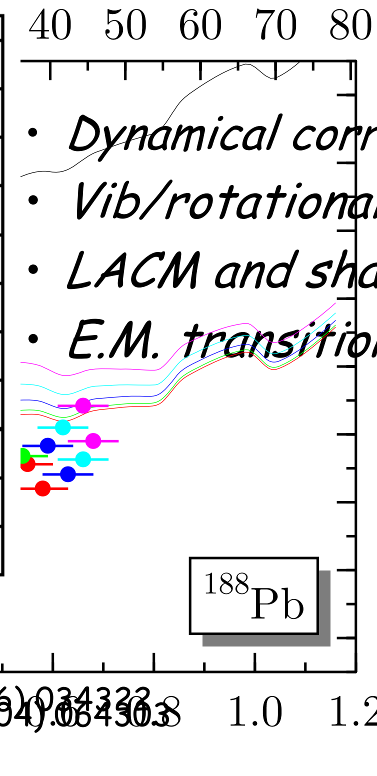
- Numerically friendly
- Mass table of deformed even-even nuclei in a few hours

M. Bender, P.-H. Heenen, P. Bonche, PRC70 (2004) 054304

# Multi-Reference = « beyond mean-field »

- Second level of implementation
- Set of mixed states ⇔ associated *transition* density matrices
- Restoration of broken symmetries + quantum collective fluctuations




- *Dynamical correlations in the g.s.*
- *Vib/rotational excitations*
- *LACM and shape coexistence*
- *E.M. transitions in the lab frame*

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

M. Bender, P. Bonche, T. D., P.-H. Heenen, PRC69 (2004) 064303

- Numerically demanding
- Systematics possible but more than 4 coll. Var. is still challenging

M. Bender, P. Bonche, T. D., P.-H. Heenen, PRC69 (2004) 064303

# Standard energy functionals

- Skyrme = **quasi-local** / Gogny = **non-local**

Skyrme = all local densities from $\rho_q$ and $\kappa_q$ up to second order in $\nabla$

$$\mathcal{E}[\rho,\kappa,\kappa^*]=\int d\vec{r}\sum_{qq'}\Big[C^{\rho\rho}_{qq'}\,\rho_q\,\rho_{q'}+C^{ss}_{qq'}\,\vec{s}_q\cdot\vec{s}_{q'}+C^{\rho\Delta\rho}_{qq'}\,\rho_q\,\Delta\rho_{q'}+C^{s\Delta s}_{qq'}\,\vec{s}_q\cdot\Delta\vec{s}_{q'}$$
$$+C^{\rho\tau}_{qq'}\left(\rho_q\,\tau_{q'}-\vec{j}_q\cdot\vec{j}_{q'}\right)+C^{J^2}_{qq'}\left(\vec{s}_q\cdot\vec{T}_{q'}-\mathcal{J}_q\,\mathcal{J}_{q'}\right)$$
$$+C^{\rho\nabla J}_{qq'}\left(\rho_q\,\vec{\nabla}\cdot\vec{J}_{q'}+\vec{s}_q\cdot\vec{\nabla}\wedge\vec{j}_{q'}\right)+C^{\nabla s\nabla s}_{qq'}\left(\vec{\nabla}\cdot\vec{s}_q\right)\left(\vec{\nabla}\cdot\vec{s}_{q'}\right)\Big]$$
$$+\sum_{q}C^{\tilde{\rho}\tilde{\rho}}_{qq}\,|\tilde{\rho}_q(\vec{r})|^2+\text{additional terms involving gradients}$$

- ***Universal*** = applicable to *all nuclei* without local adjustment
- ***Empirical*** = no link to NN/NNN + fitted on experimental data
- Simplistic density-dependent couplings
- Similar good performances for properties of known nuclei
- "Asymptotic freedom" as one jumps into the ***next major shell***

# Which theoretical method(s)?

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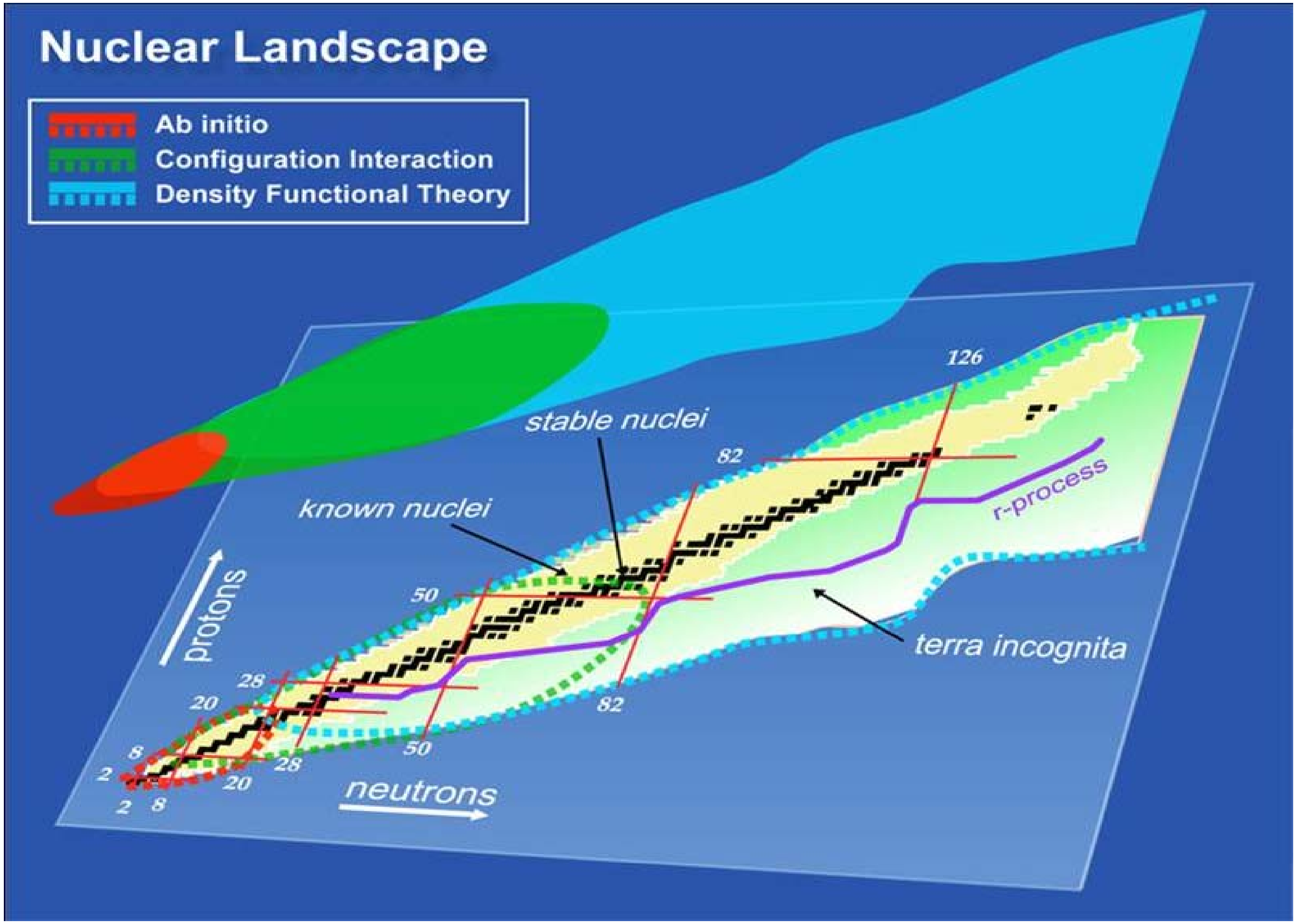


- No "one size fits all" theory for nuclei
- All theoretical approaches need to be linked eventually