Mean Field and beyond: Progress and challenges in describing medium and heavy nuclei

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Nuclear Structure 12

My selection

1. Improvement of the EDF/performance
2. Microscopic Bohr Hamiltonian
3. Non-adiabatic description of yrast states
4. Combination of EDT with shell model
5. Level densities from SMMC calculations

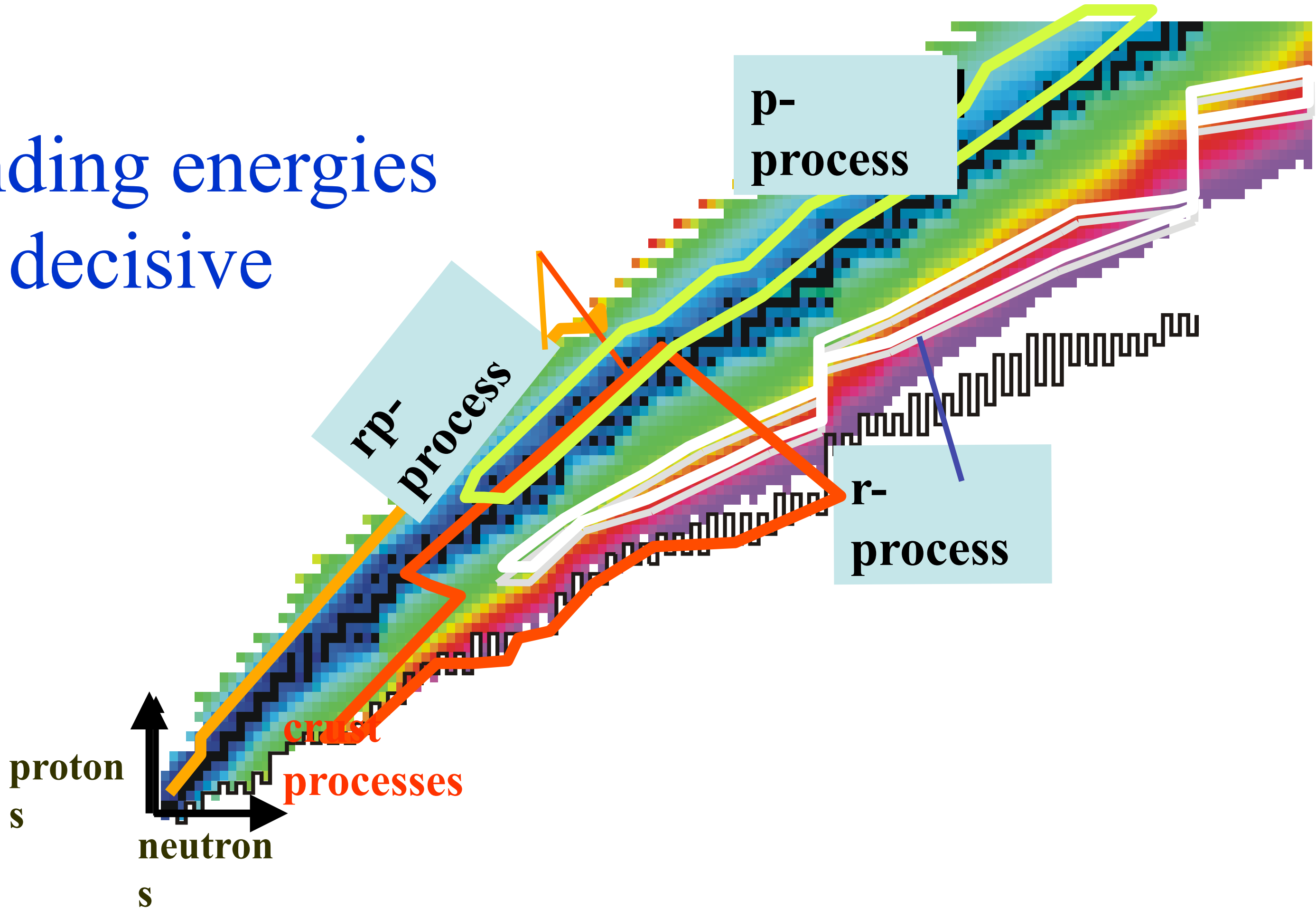
New level of computation

Access to supercomputing
Massive parallel processing
SciDAC in US
CompStar in EU
RIKEN in Japan
…

-Deformed nuclei are included in the optimization of the EDF functionals.
-Mass tables are easily produced.
-Full RPA calculations deformed nuclei have been carried out.
-Low lying collective excitations are calculated for all bound nuclides.
-Shell Model Monte Carlo calculations of level densities

1. Improvement of the EDF/ performance

Binding energies are decisive



Mean field:

$V(\vec{r},\sigma,\tau), V_{ls}(\vec{r},\sigma,\tau), \Delta(\vec{r}), \ldots$

observables

Solution of the HFB eqs.,

(Schroedinger/Dirac)

quasiparticle energies, amplitudes

density matrix, pairing tensor

$\rho_{T=0,1}(\vec{r},\sigma;\vec{r}',\sigma'); \kappa_T(\vec{r},\sigma;\vec{r}',\sigma')$

local densities and currents

$\rho_{T=0,1}(\vec{r}), s_T(\vec{r}), \vec{j}_T(\vec{r}), \ldots$

Selfconsistency:

Skyrme EDF, PC-RMF EDF,

FR-RMF, Gogny interaction,

FRDM (incomplete sc.)

parameters

experiment

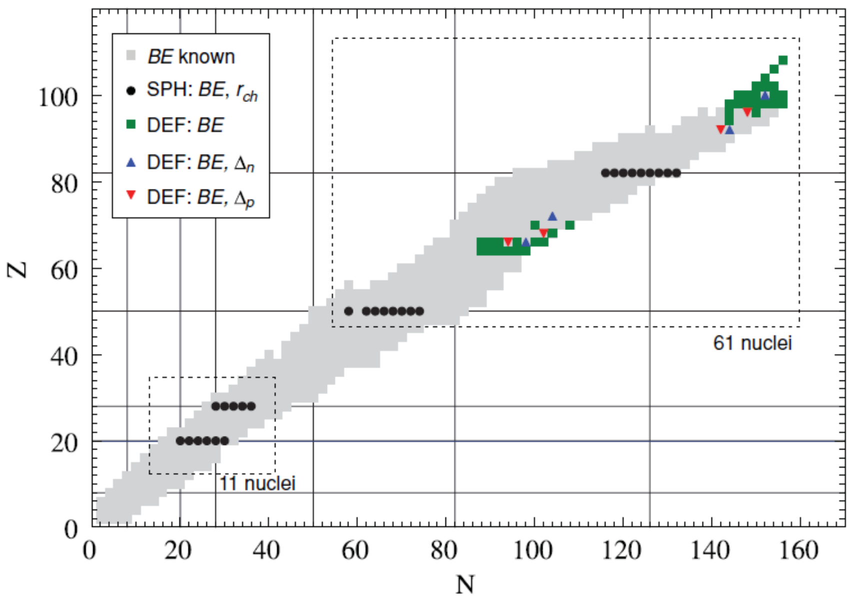
nucl. matter calcs.

Skyrme EDF

$$E = \sum_{T=0,1} \int d^3r \left[e_{kin}(\vec{r}) + e_{\text{int}}[\rho_T(\vec{r}), \vec{J}_T, ..] + e_{Coul}(\vec{r}) + e_{pair}[\kappa_T(\vec{r})] \right]$$

Mean field : functional derivative with respect qp. amplitudes

UNEDF collaboration
UNEDF0: M. Kortelainen et al. PRC 82, 024313 (2010)
12 parameters for Skyrme EDF + 2 pairing strengths

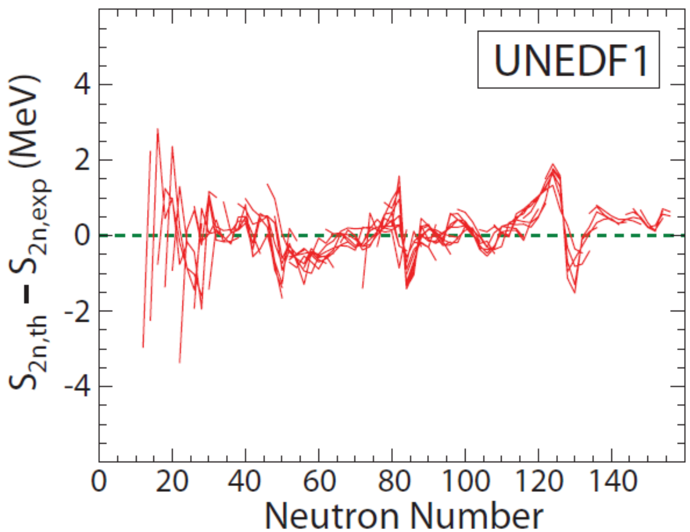


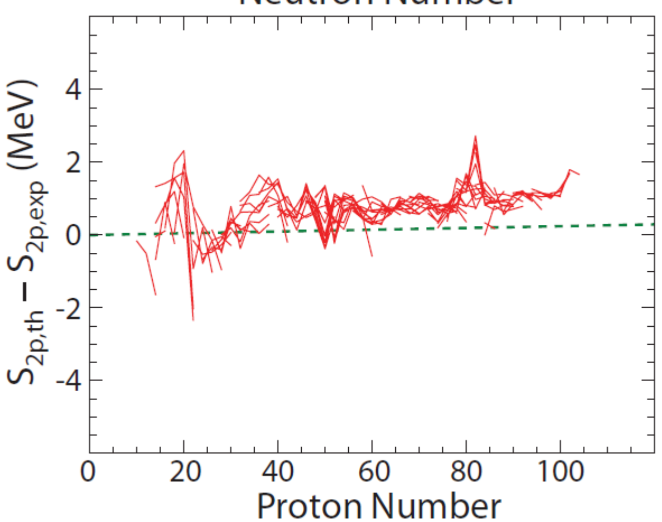
Fit protocol:

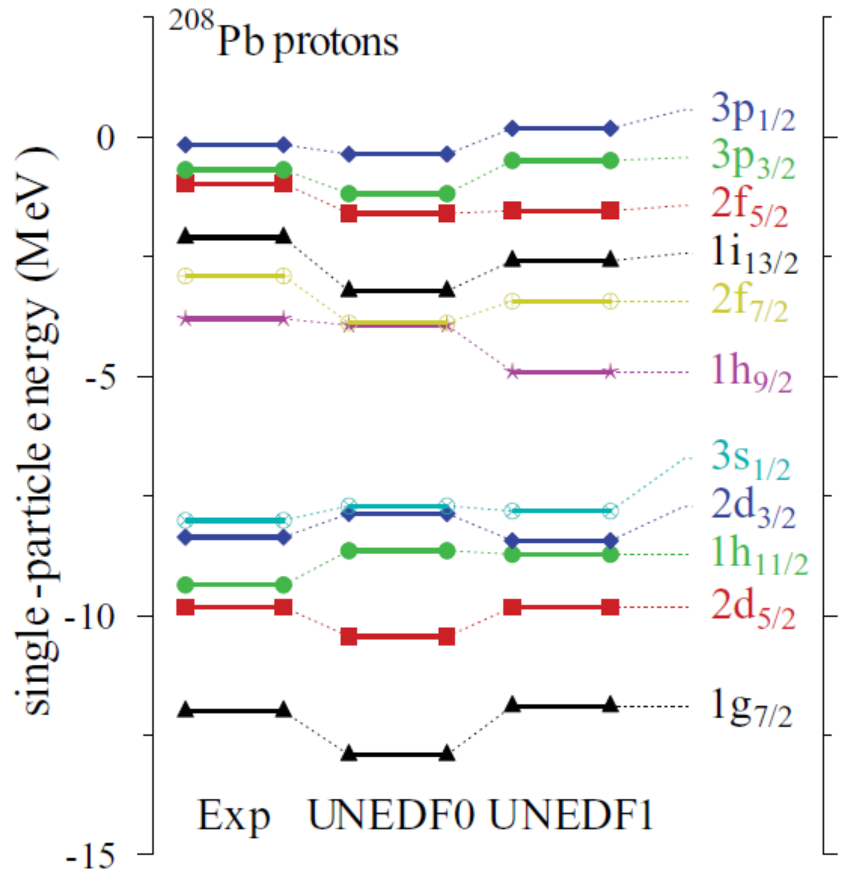
72 carefully chosen nuclei
Energies, radii
Bonds on nuclear matter

ρ_c	[+0.15,+0.17]
E^{NM}/A	[−16.2,−15.8]
K^{NM}	[+190, +230]
$a_{\text{sym}}^{\text{NM}}$	[+28, +36]
$L_{\text{sym}}^{\text{NM}}$	[+40, +100]
$1/M_s^*$	[+0.9, +1.5]

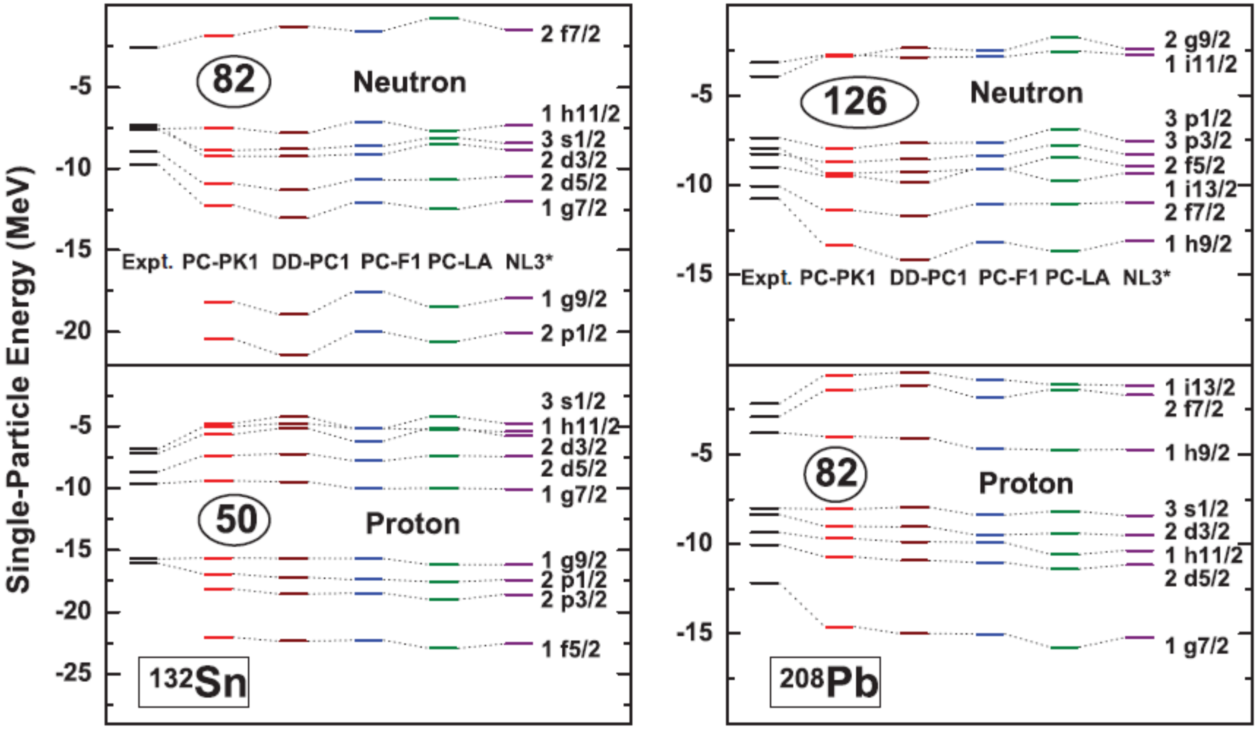
UNEDF1: M. Kortelainen et al. PRC 85, 024304 (2012)
Excitation energies of fission isomers added to fit







RMSD(mass) = 1.455MeV, RMSD(radii) = 0.016 fm, and RMSD(OES) = 59 keV.
M^*=0.9M very good sp spectra



RMF: Relativistic Mean Field
PC: Point Coupling
Beijing group PC-PK1:
P. W. Zhao et al. PRC 82, 054319 (2010)

RMSD(mass) = 1.4MeV

Spacing of the sp. levels reflects effective mass $M^*/M \sim 0.7$

The effective mass challenge:

-$M^*/M \sim 1$ gives correct spacing of the single particle levels around Fermi level, crucial for mass predictions better than 0.8 MeV, FRDM example

-$M^*/M \sim 0.8$-0.9 ab initio calculations of nuclear matter

-$M^*/M \sim 0.8$ Giant Quadrupole Resonance

Suggested solution: particle vibration coupling : see E. Litvinova’s, A. Afanasjev’s talks

$M^*/M \sim 1$ just an accident?

Mean field:

$V(\vec{r},\sigma,\tau), V_{ls}(\vec{r},\sigma,\tau), \Delta(\vec{r}),\ldots$

Solution of the HFB eqs.,

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Selfconsistency:

Skyrme EDF, PC - RMF EDF,

FR - RMF, Gogny interaction,

FRDM (incomplete sc.)

observables

parameters

phenomenological

corrections:

-Wigner term

-quadrupole

correlations

experiment

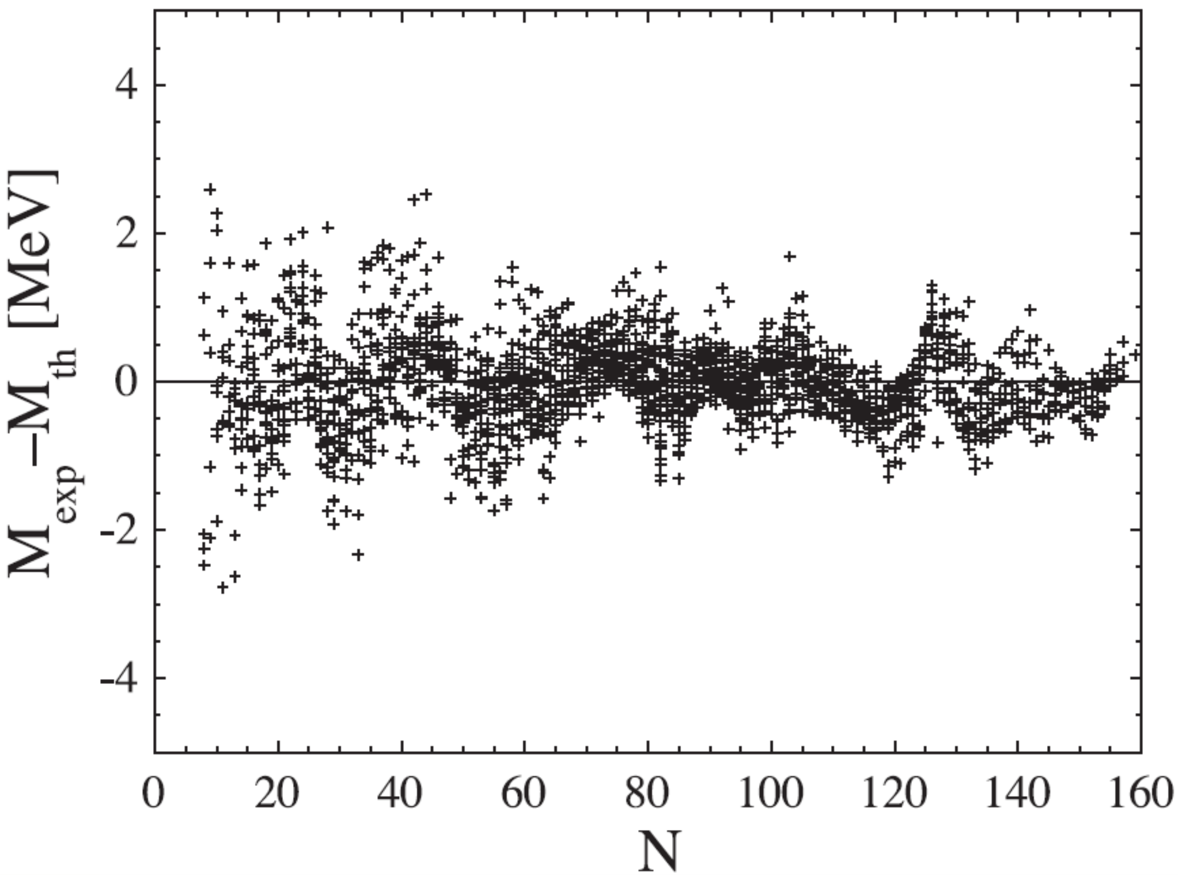
nucl. matter calcs.

parameters

Skyrme EDF with corrections

BSk17-21 EDF
+ phenomenological Wigner term (extra binding of N=Z nuclei)
+phenomenological quadrupole correlations
(shape fluctuations, rotational symmetry restoration)
+pairing cut off energy as a fit parameter

Brussels- Montreal collaboration
HFB-17: S. Goriely et al. PRL 102, 152503 (2009)
24 parameters, Fit protocol includes:
2149 experimental masses, properties of symmetric N. M. and neutron matter, exp. giant resonances, pair gap of N. M.



σ(2144 nuclides) = 0.58 MeV

47% of gs. spins and

72% of gs. parities

of odd nuclei correctly predicted

reasonable level densities

(combinatorial method)

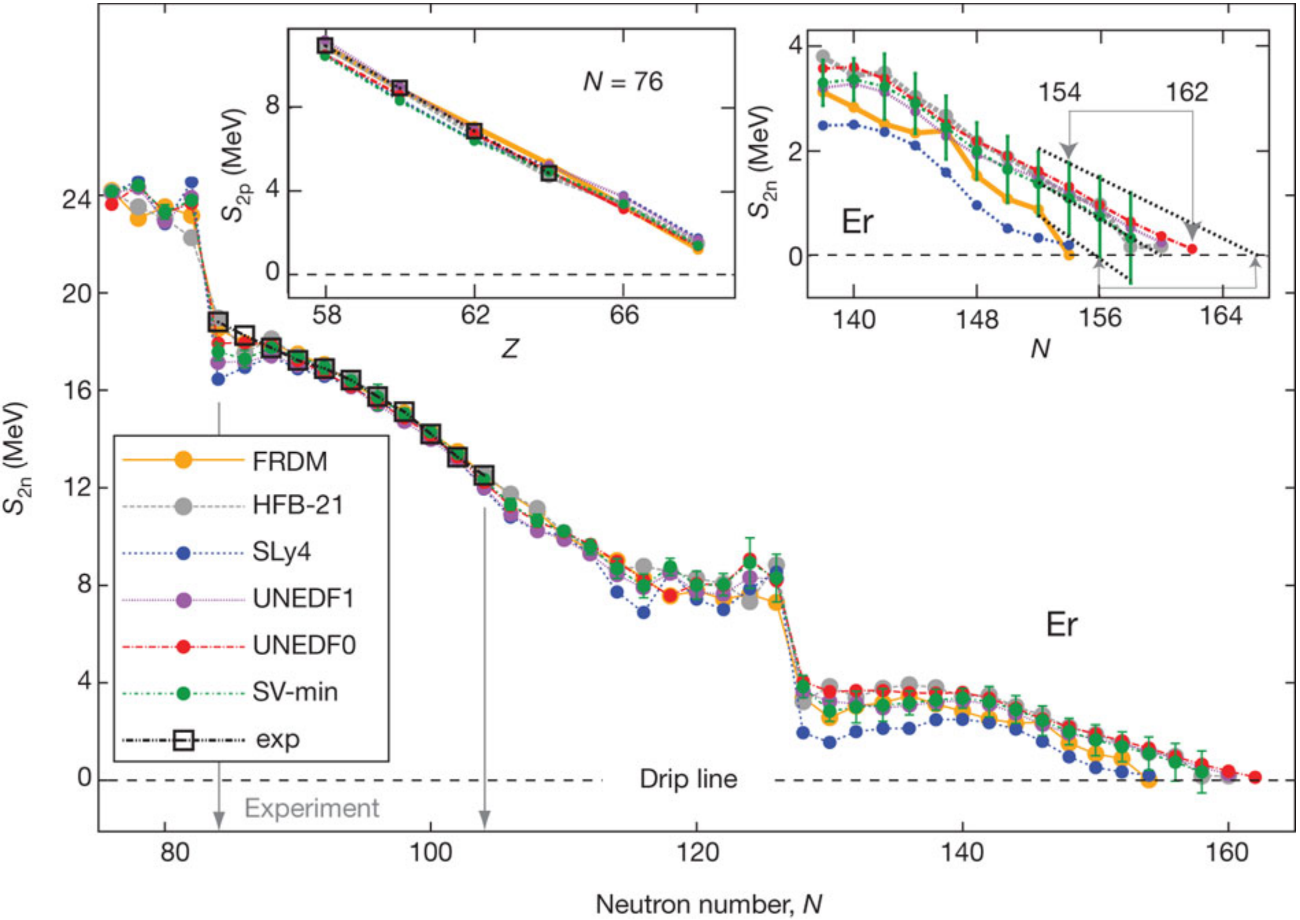
Brussels- Montreal collaboration

HFB-19 –HFB-21: S. Goriely et al., PRC 82, 035804 (2010),

25 parameters,

extra term in Skyrme EDF to get spin susceptibility right

Fit protocol: similar to HFB17, three many-body calculations for neutron matter, similar performance as HFB17



J. Erler *et al.* *Nature* **486**, 509-512 (2012)

Calculated and experimental two-neutron separation energies of even–even erbium isotopes.

EDF: RMSD 1.4MeV → improve the functional (Effective Field Theory)

+correction: RMSD 0.6MeV → calculate corrections (correlations beyond mf.)

Most important phenomenological corrections:

Wigner term –
extra binding of $N \approx Z$ nuclei: isovector pair correlations
I. Bentley, S. Frauendorf
arXiv: 1202:2795

Long range correlations of quadrupole type

2. Microscopic description of quadrupole collectivity – adiabatic approaches

Adiabatic separation of the slow collective quadrupole motion from the fast quasiparticle particle motion.
Existence of a substantial pair gap is crucial.

EDF + constraints to fix the shape Q_{20}, Q_{22} or β,γ

TDHF +quantization

Bohr Hamiltonian
$$H(\beta,\gamma) = T_{rot}(\beta,\gamma) + T_{vib}(\beta,\gamma) + V(\beta,\gamma)$$

GCM+GOA

Diagonalization

Hill - Wheeler equations
$$\sum_{q'} f_{q'} \langle q | H - E | q' \rangle = 0$$

ground state correlations: energies, radii
energies and B(E2) of excited states

Bordeaux -Brussels – Seattle collaboration:
M. Bender et al. PRC 78, 054312 (2008)

smoothing of $E_0(N,Z)$

E_{2^+} too large

Microscopic Bohr Hamiltonian

RMF EDF PC-F1
+ BCS pairing with delta force
+Cranking mass parameters
Beijing-Zagreb collaboration:
Example: Z. K. Li et al. PRC 81, 034316 (2010)

Selected regions
of transitional nuclei

Sly4 EDF
+ BCS pairing with delta force
+Cranking mass parameters
Warsaw group:
Example: H. Watanabe et al. PLB 704, 270 (2011)

Selected regions
of transitional nuclei

Gogny interaction (ph and pp channel)
+sc. cranking moments of inertia
+cranking shape mass parameters
+zero point energy correction (GOA)
Bruyères le Châtel – Seattle collaboration

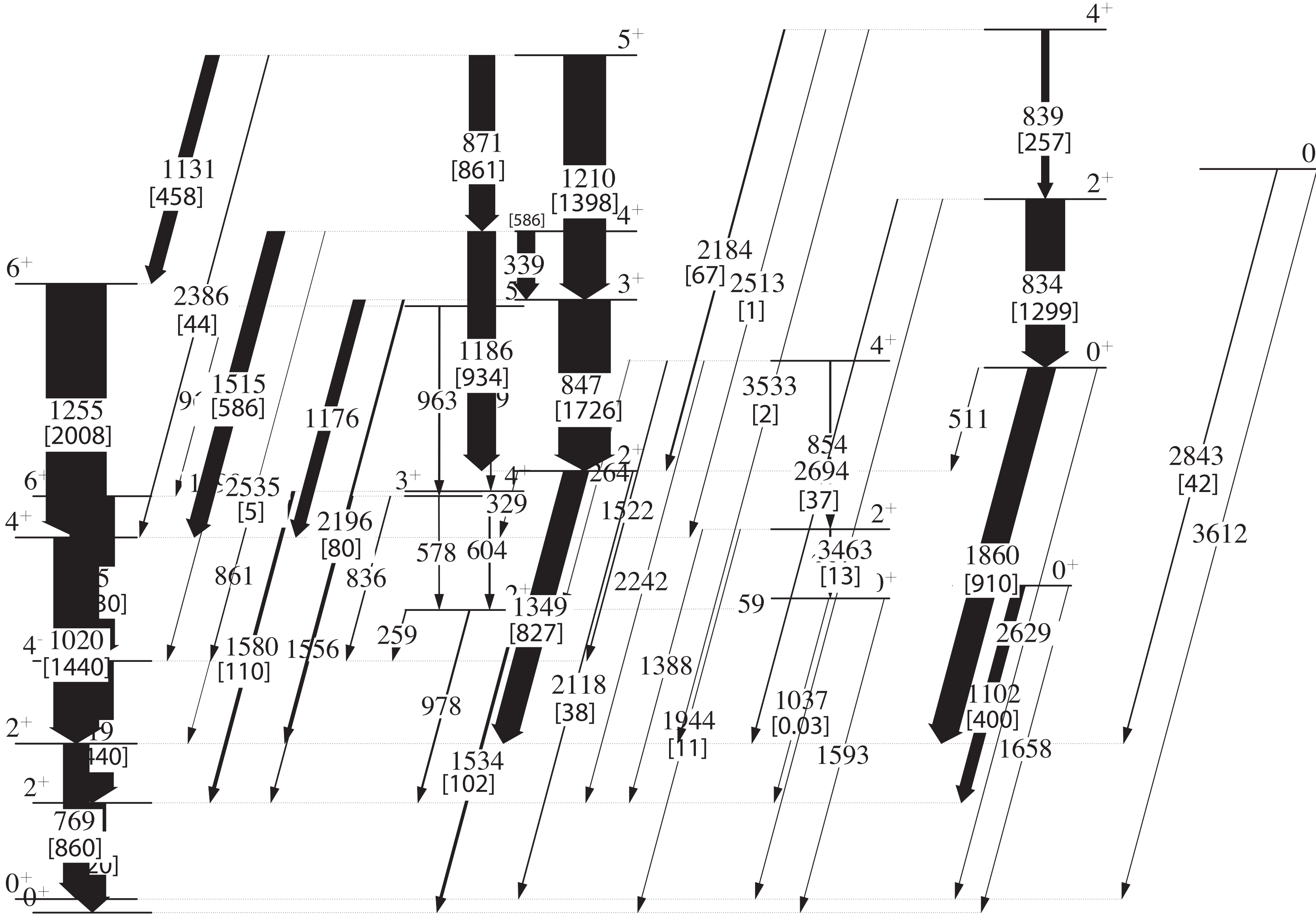
J.-P. Delaroche et al. PRC 81, 014303 (2010)

Benchmark calculation across the mass table 1700 e.-e. nuclei.
Energies and BE2 0^+_1, 2^+_1, 4^+_1, 6^+_1, 0^+_2, 2^+_2, 2^+_3 tabulated.

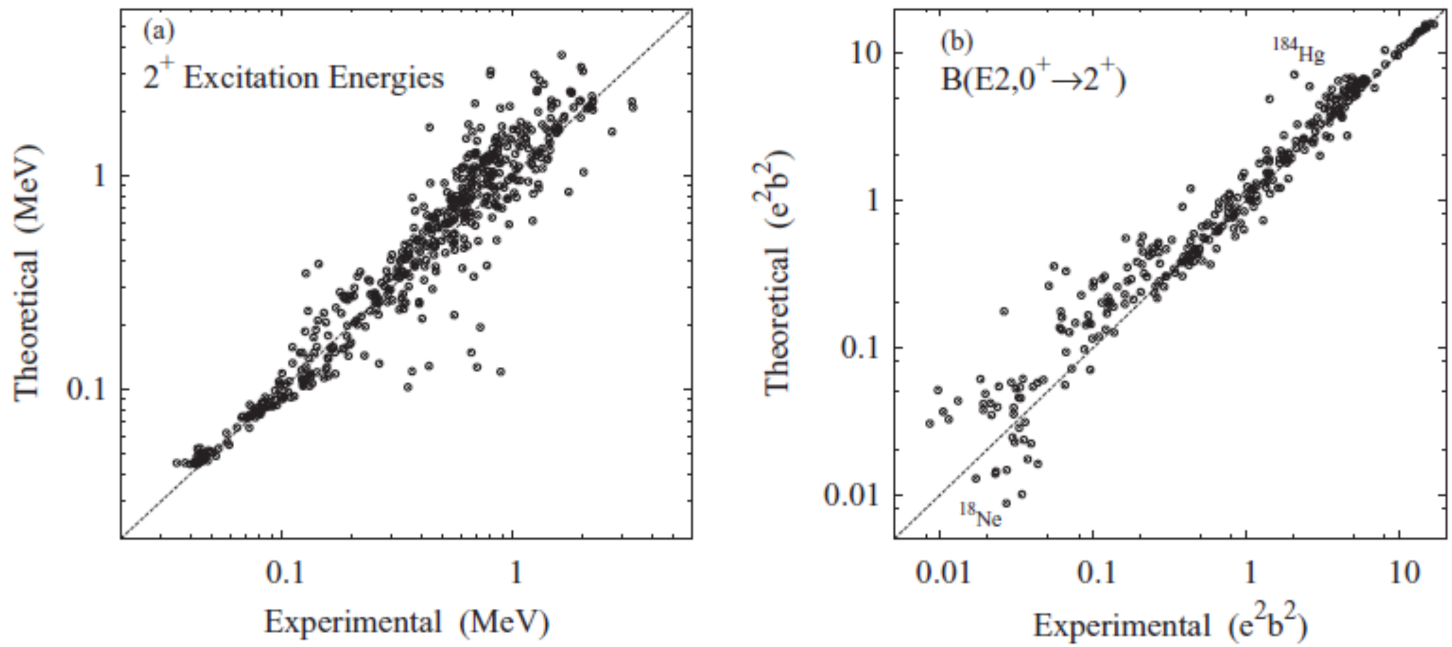
Influence of the long range correlations on binding energies comparable to GCM of Bordeaux -Brussels – Seattle collaboration.

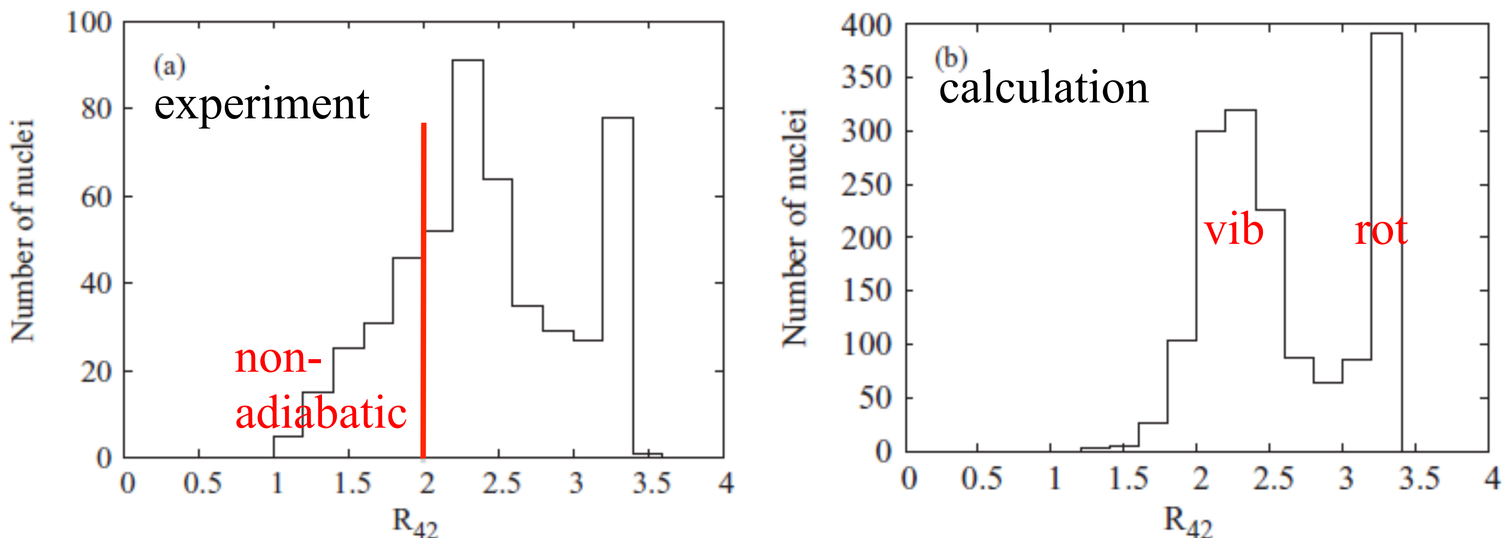
Careful analysis of performance

^{102}Pd Experiment / Microscopic Bohr Hamiltonian



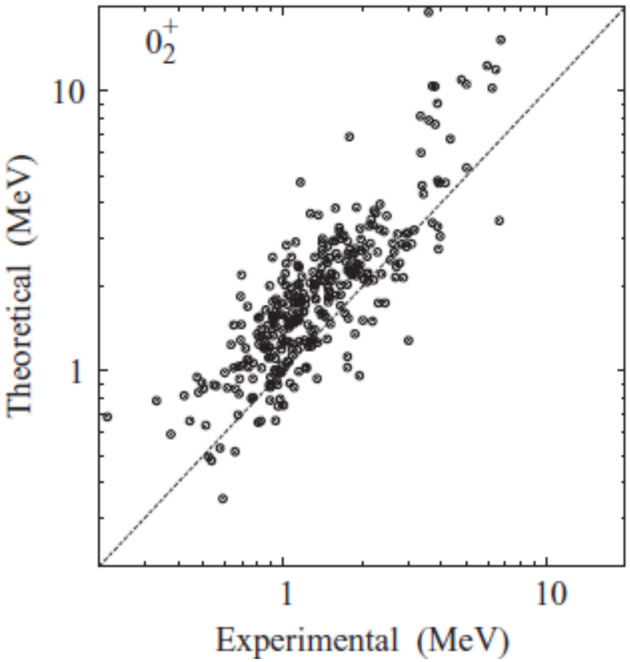
Yrast states 2^+_1 and 4^+_1 well described



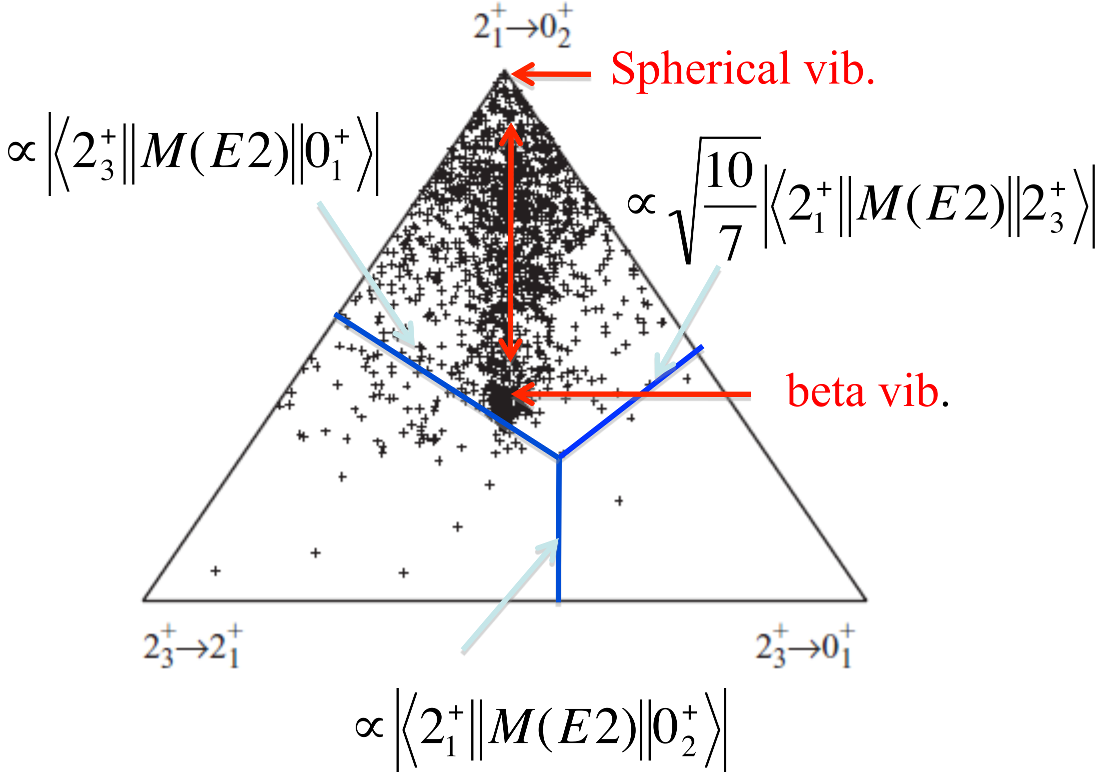


$$R_{42} = \frac{E(4_1^+)}{E(2_1^+)}$$

The 0^+_2 problem



too high



The 0^+_2 states do not have beta vib. character

P. E. Garrett,
J. Phys. G: Nucl. Part. Phys. **27** **(2001) R1**

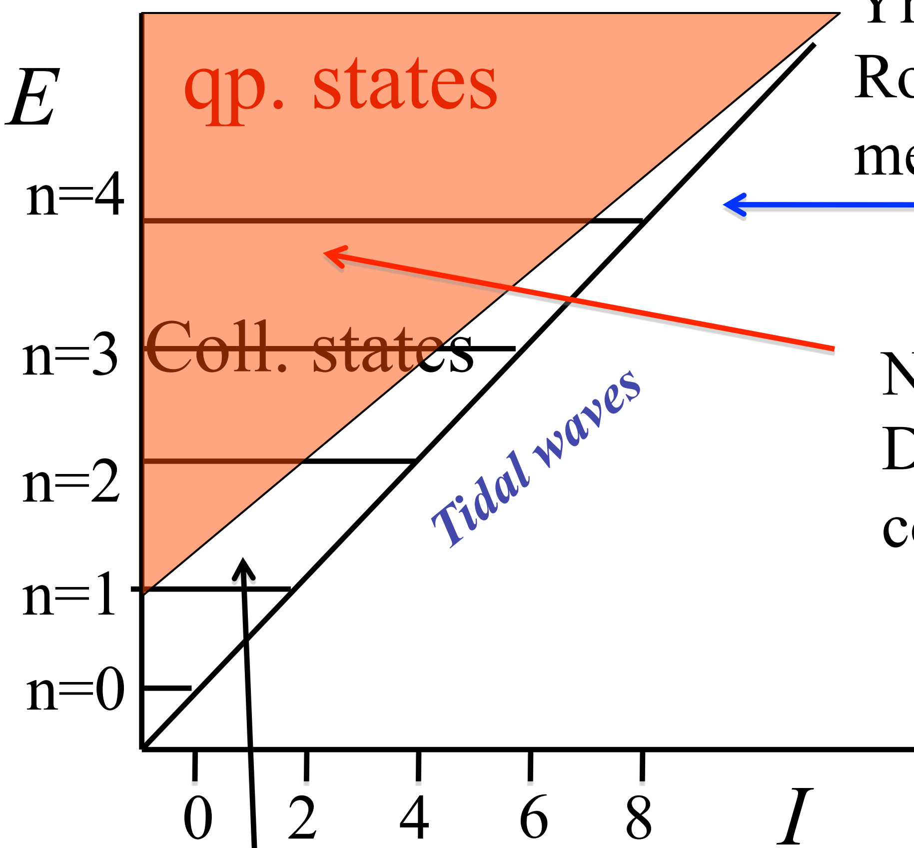
calculation too vibrational

For example:

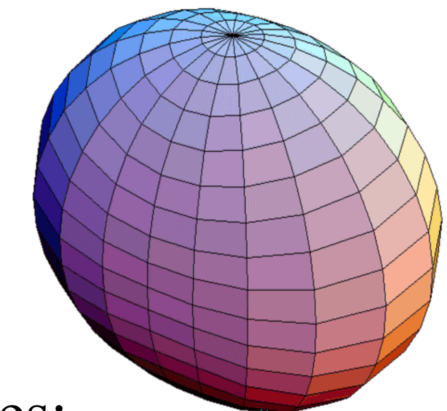
experimental B(E2, 2^+_1->0^+_2) much smaller

Adiabatic approximation problematic

Beyond the adiabatic approximation



Yrast states:
Rotating
mean field



Non-yrast states:
Diagonalization of
configuration interaction

Adiabatic region

How describe the non-adiabatic region?

3. Non-adiabatic description of yrast states

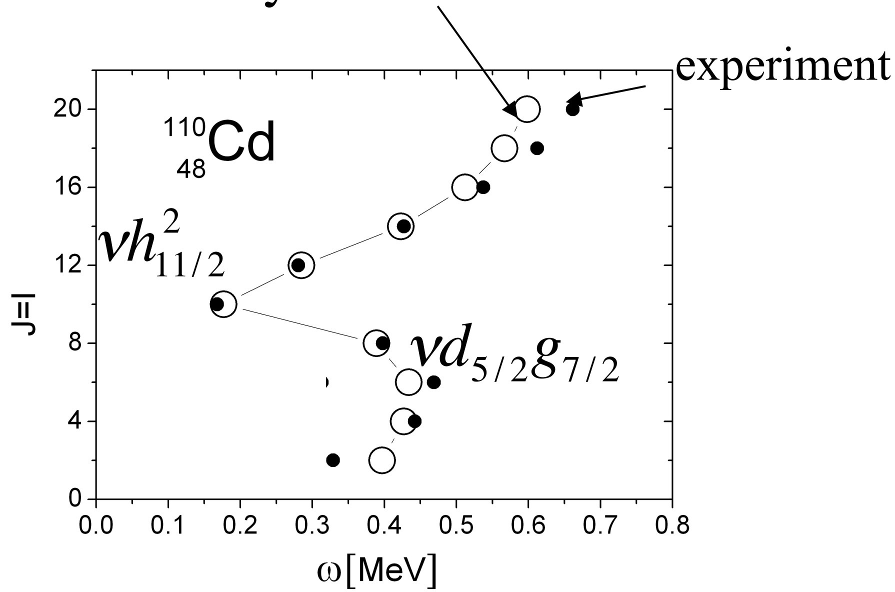
Tidal waves

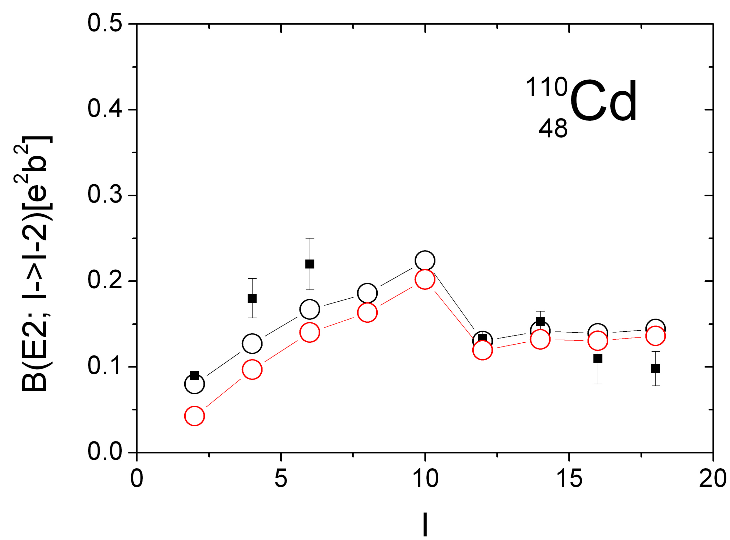
non-adiabatic semiclassical treatment: mean field with constraint $-\omega J_x$

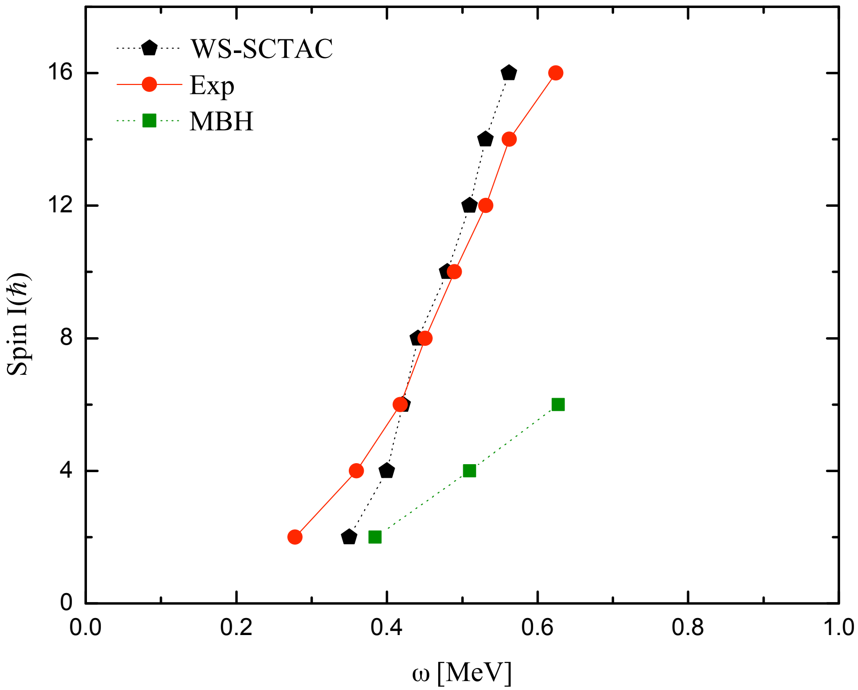
UND Frauendorf, Gu, Sun, IJMP E **20** 465 (2011), arXiv: 0709.025

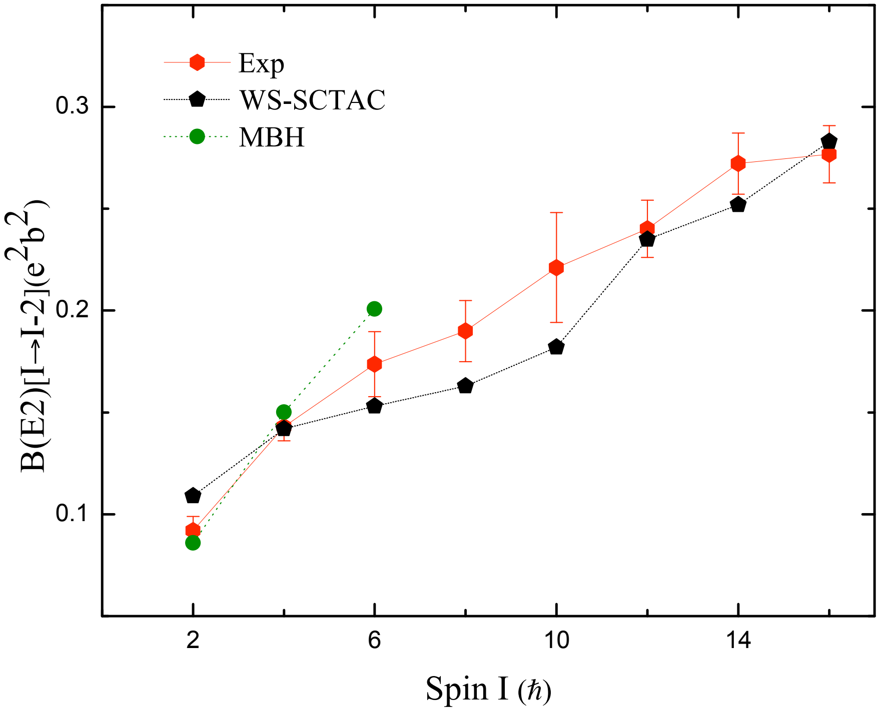
Cranking Micro-Macro with Woods Saxon

Works for the yrast states of vibrational nucleus!









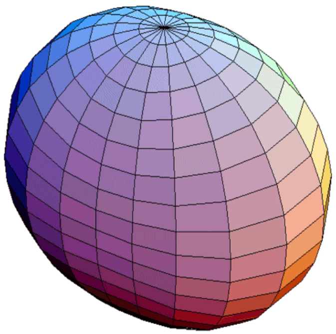
WS - TAC : Cranking Micro - Macro with Woods Saxon

Works well for the yrast states of transitional ^{102}Pd

No quantal shape fluctuations

MBH : Microscopic Bohr Hamiltonian

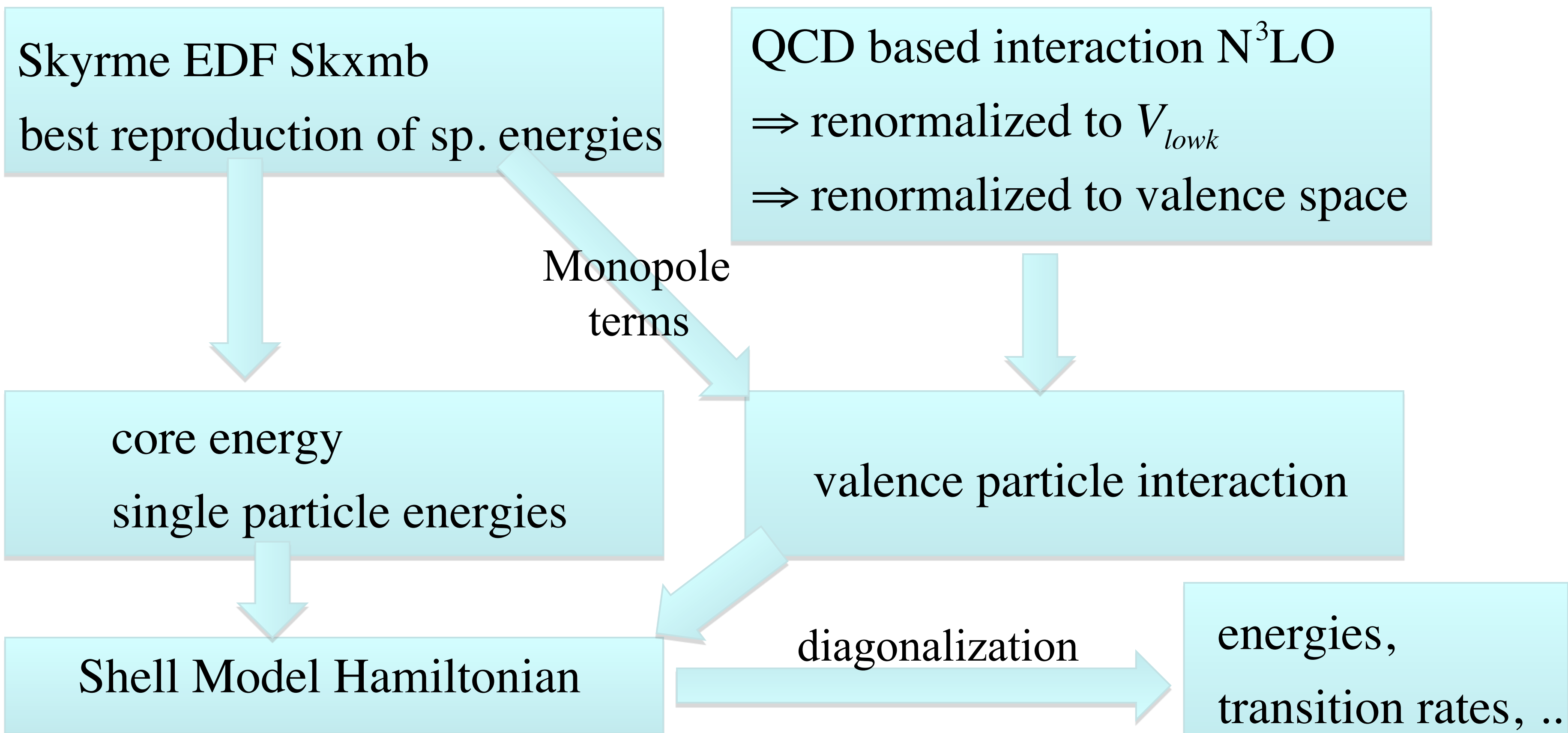
Fully quantal but adiabatic

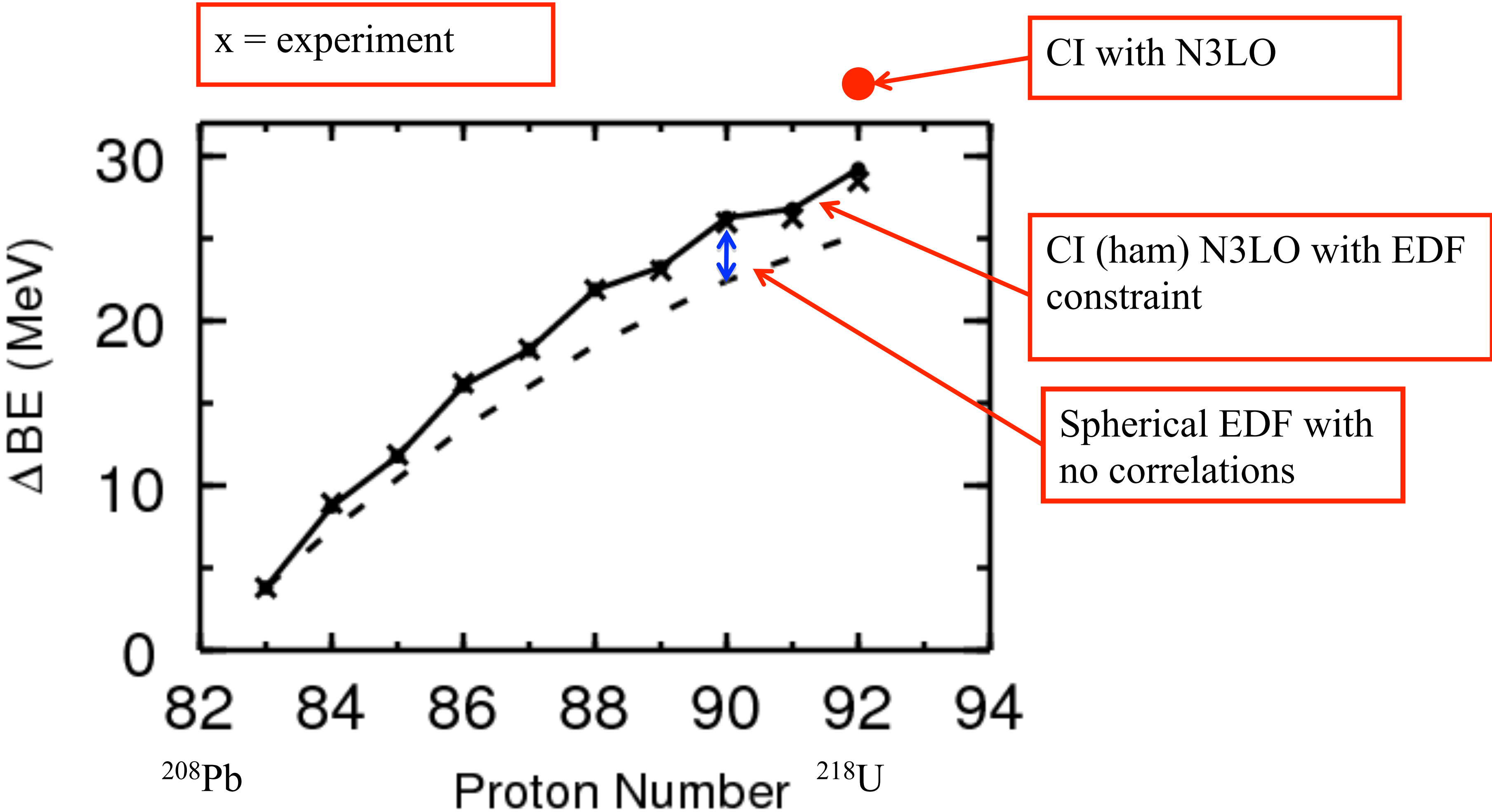


See poster by Daniel Ayangeakaa et al.
Notre Dame + Argonne

4. Combination of EDF with configuration mixing

MSU-Oslo collaboration
Brown, Signoracci, Hjorth-Jensen, PLB 695, 507 (2011)

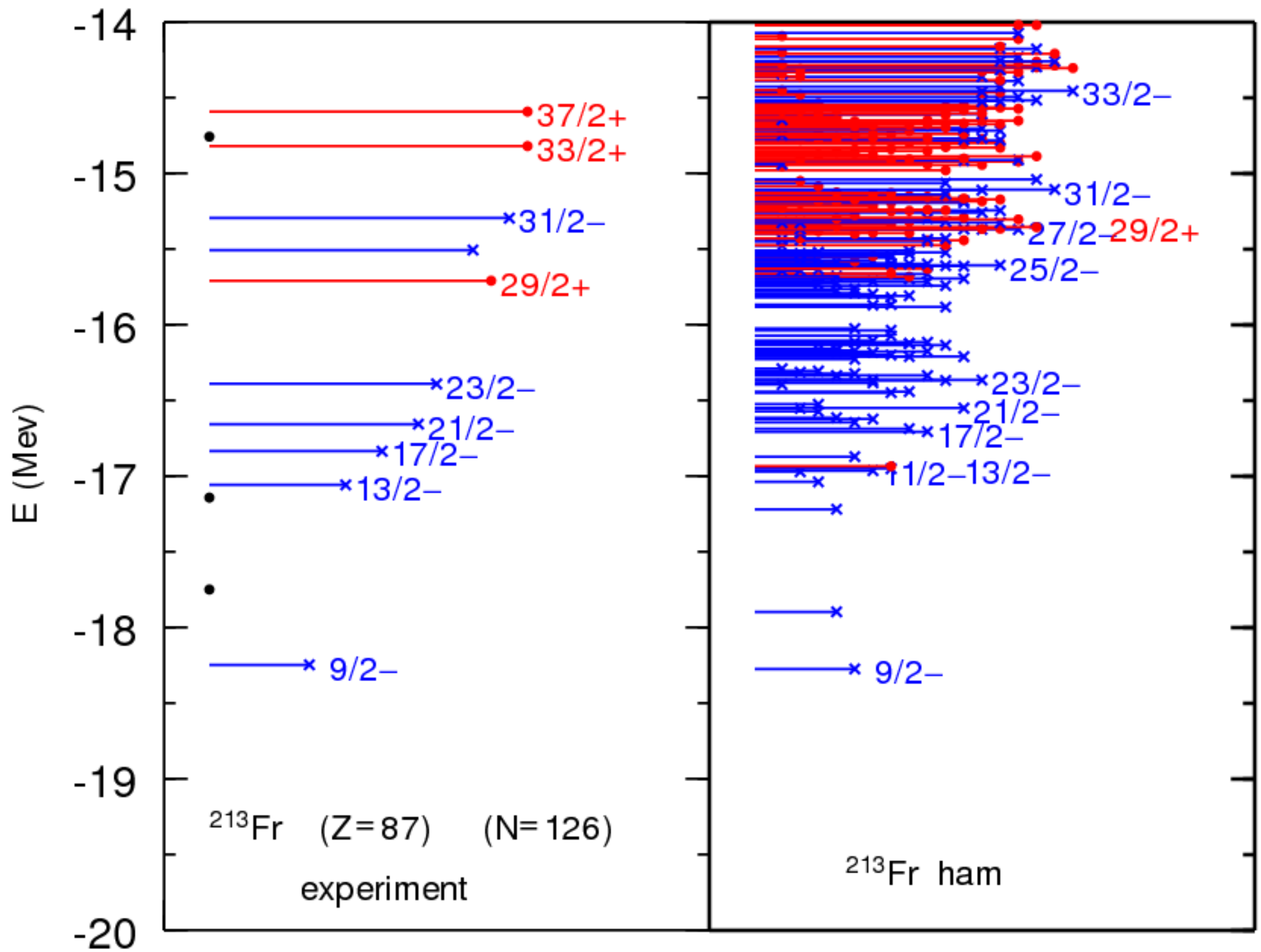




Correlations beyond spherical mean field (dynamical deformation +???) lead to accurate binding energies.

Courtesy B. A. Brown

"ab-initio" calculation for absolute energies of ^{213}Fr



Most accurate prediction for a heavy open shell nucleus

Courtesy B. A. Brown

5. Shell Model Monte Carlo for level densities

C. ¨Ozen, et al. arXiv:1206;6773
Istanbul-Yale-Chiba collaboration

Mean field
Woods - Saxon, Sly4
δ - pairing

mapping →

single particle energies
multipole - multipole interaction
$\lambda = 0, 2, 3, 4$

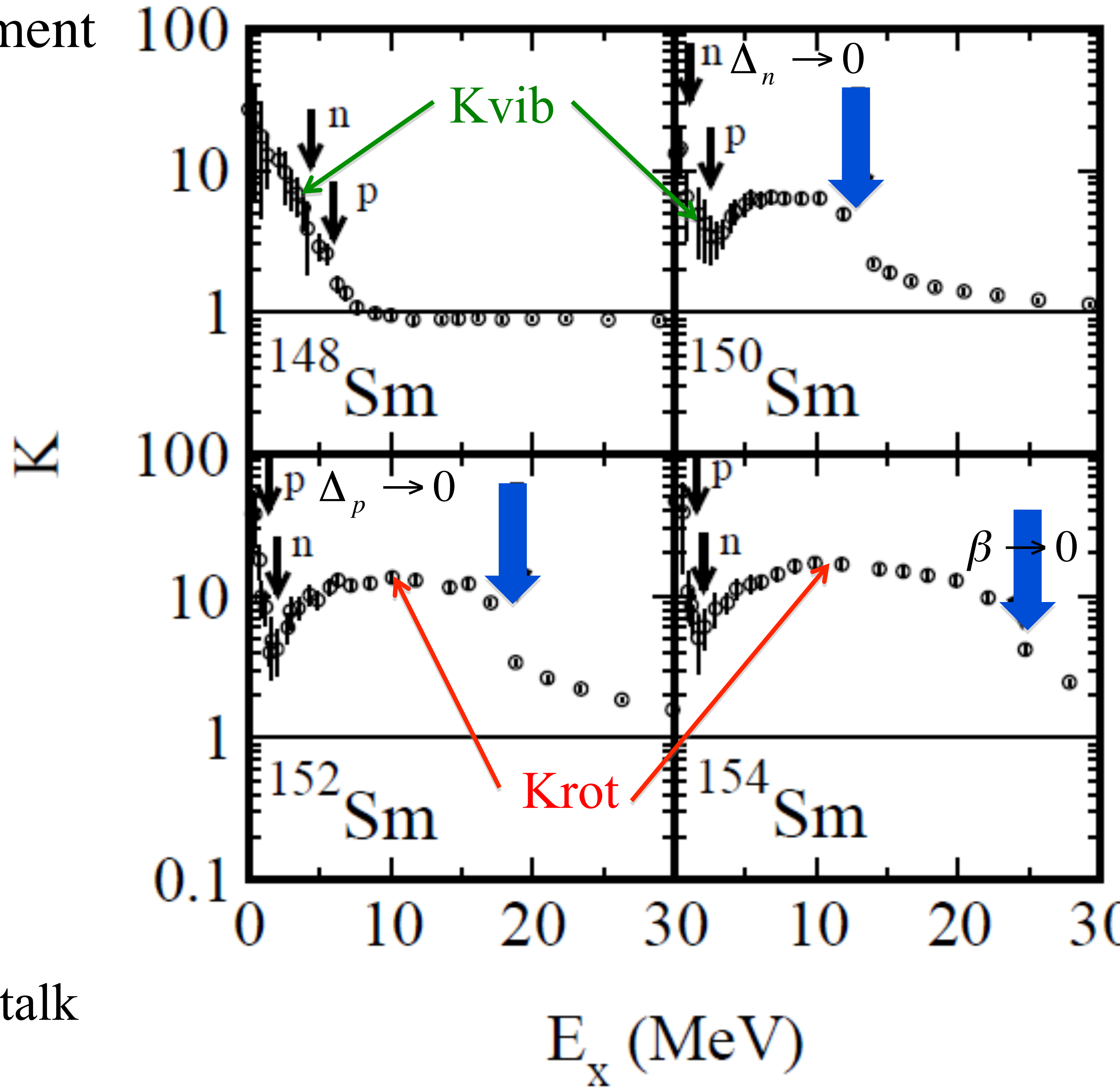
↓ SMMC

thermal properties :
partition function (canonical)
state density
parity ratio, $< J^2 >$, ...

collective enhancement

$$K = \frac{\rho_{correlated}(E_x)}{\rho_{mean\ field}(E_x)}$$

presence of vibrational and rotational states



So far:
phenomenological
K- correction
T dependence?
First calculation
See also Dossing's talk

Summary/Outlook

- Accuracy of mean field ground state energies ~1.4MeV, with phenomenological corrections ~0.6MeV
- Is it possible to construct better functionals? How to calculate the corrections beyond mean field?
- Adiabatic treatment of quadrupole degrees of freedom reasonably well describes 2^+_1, 4^+_1, 2^+_2 states across mass table. Higher states in e-e nuclei, most states in odd-A non-adiabatic.
- How to treat the non-adiabatic excitations?
  Rotating mean field for yrast states
  Combination of mean field methods with shell model configuration mixing for non-yrast states.
- Shell Model Monte Carlo method accounts for vibrational and rotational enhancement of level densities.

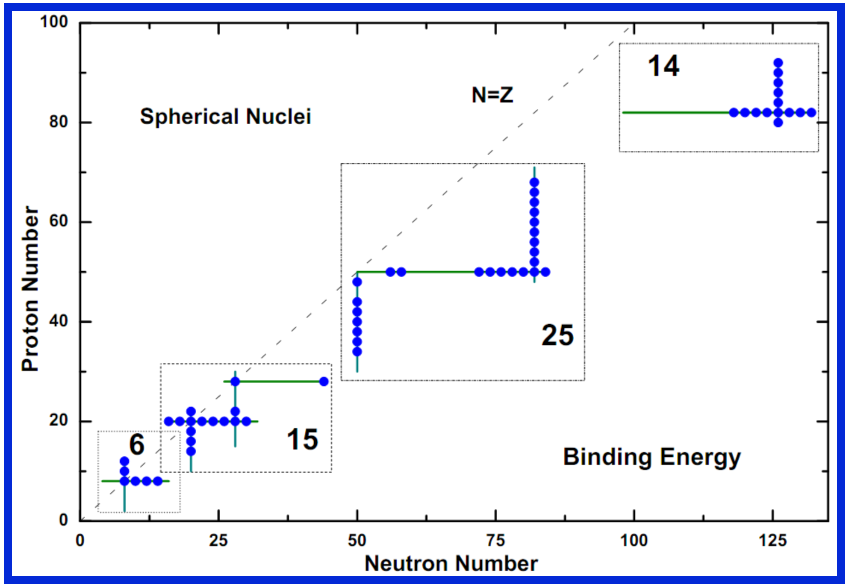
Backup slides

Relativistic Mean Field
Point coupling EDF: PC-RMF

$$E = \int d^3r \left[e_{kin}(\vec{r}) + e_{\text{int}}[\rho_S(\vec{r}), j_V^\mu(\vec{r}), j_{TV}^\mu(\vec{r})] + e_{Coul}(\vec{r}) + e_{pair}[\kappa_T(\vec{r})] \right]$$

Mean field: functional derivative with respect qp. amplitudes

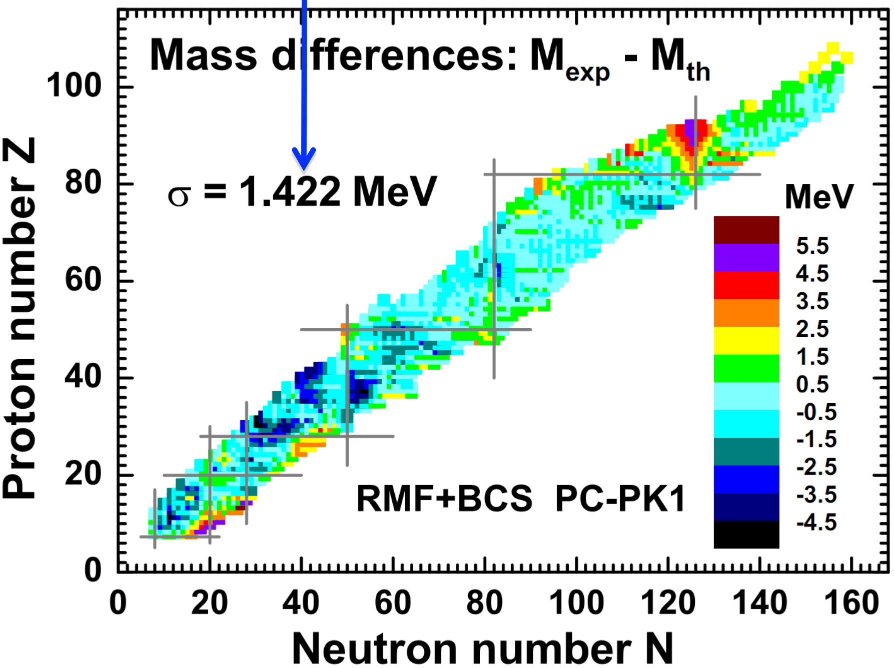
Beijing group
PC-PK1: P. W. Zhao et al. PRC 82, 054319 (2010)
9 parameters for PC-RMF EDF + 2 pairing strengths

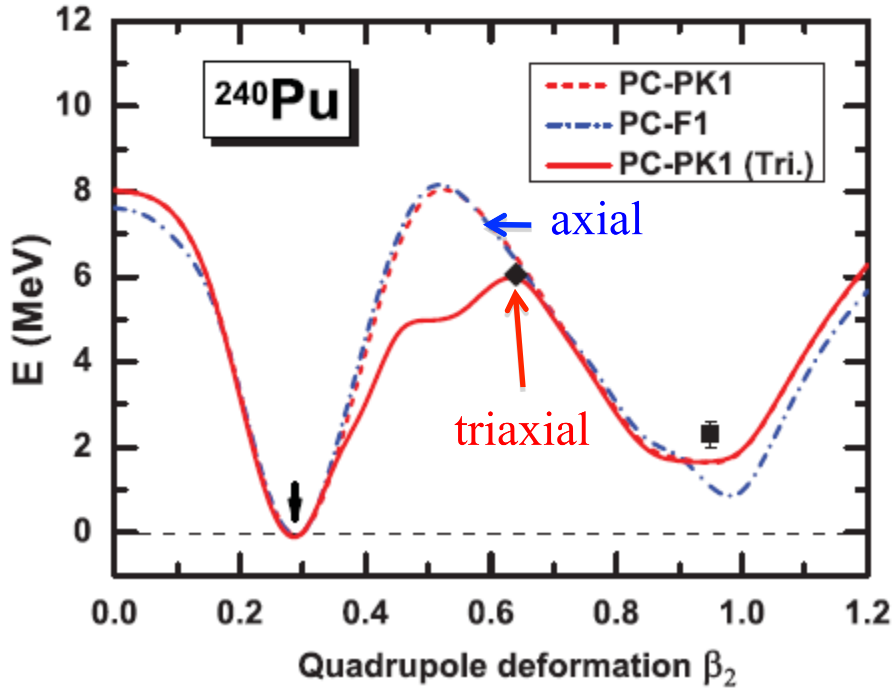


Fit protocol:

80 spherical nuclei: energies,
20 spherical nuclei: radii

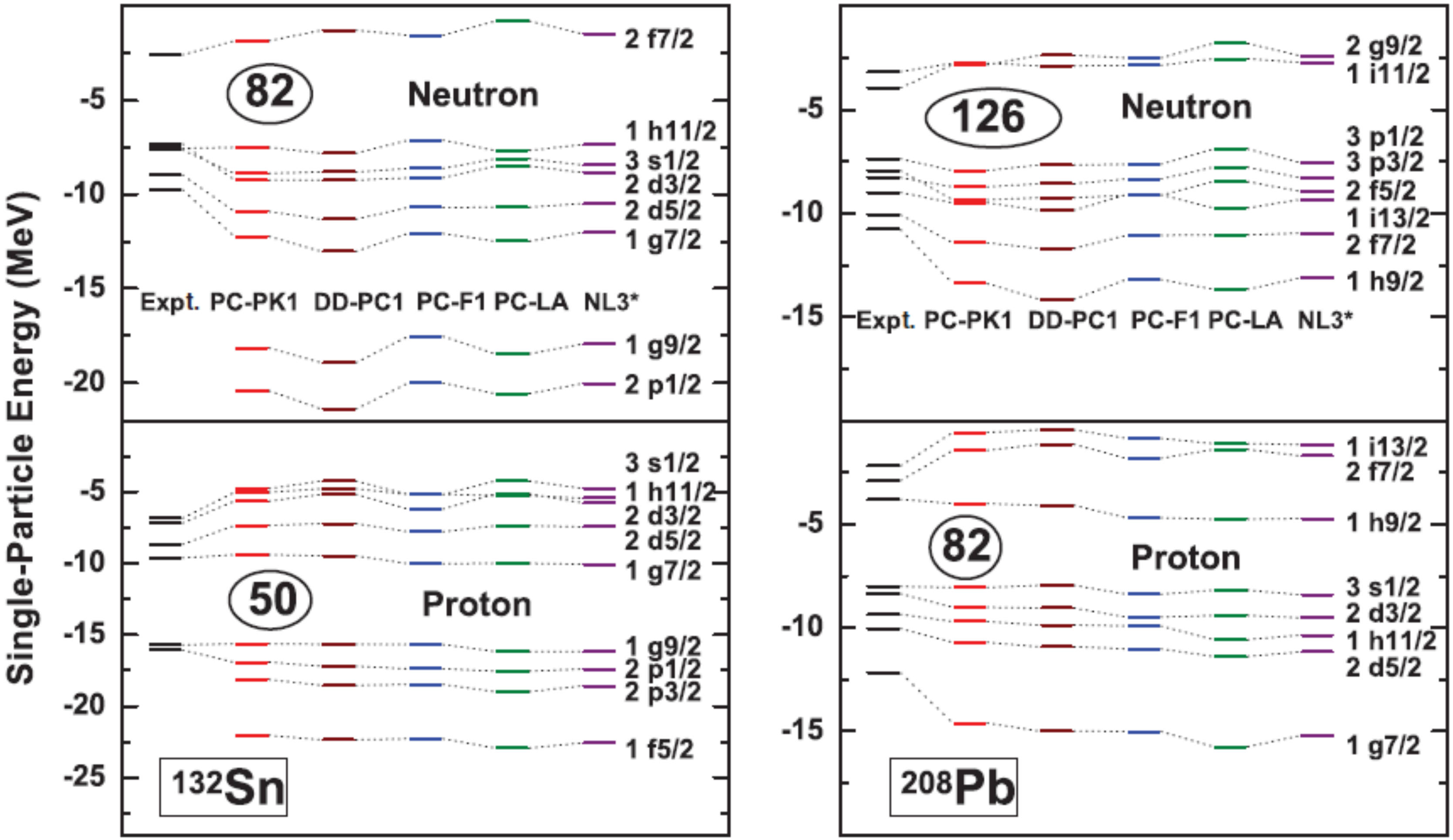
Root mean square deviation of calculated binding energies from experiment





Nuclear matter properties very well reproduced – not included in fit.

Model	ρ_0 (fm^{-3})	E/A (MeV)	M^*_D/M	M^*_L/M	E_{sym} (Mev)	L (MeV)	K_{sym} (MeV)	K_0 (MeV)	K_{asy} (MeV)
Empirical	0.166	−16	0.55 − 0.60	0.8	∼ 32	88		240	−550
	±0.018	±1		±0.1		±25		±20	±100
PC-PK1	0.153	-16.12	0.59	0.65	35.6	113	95	238	-582



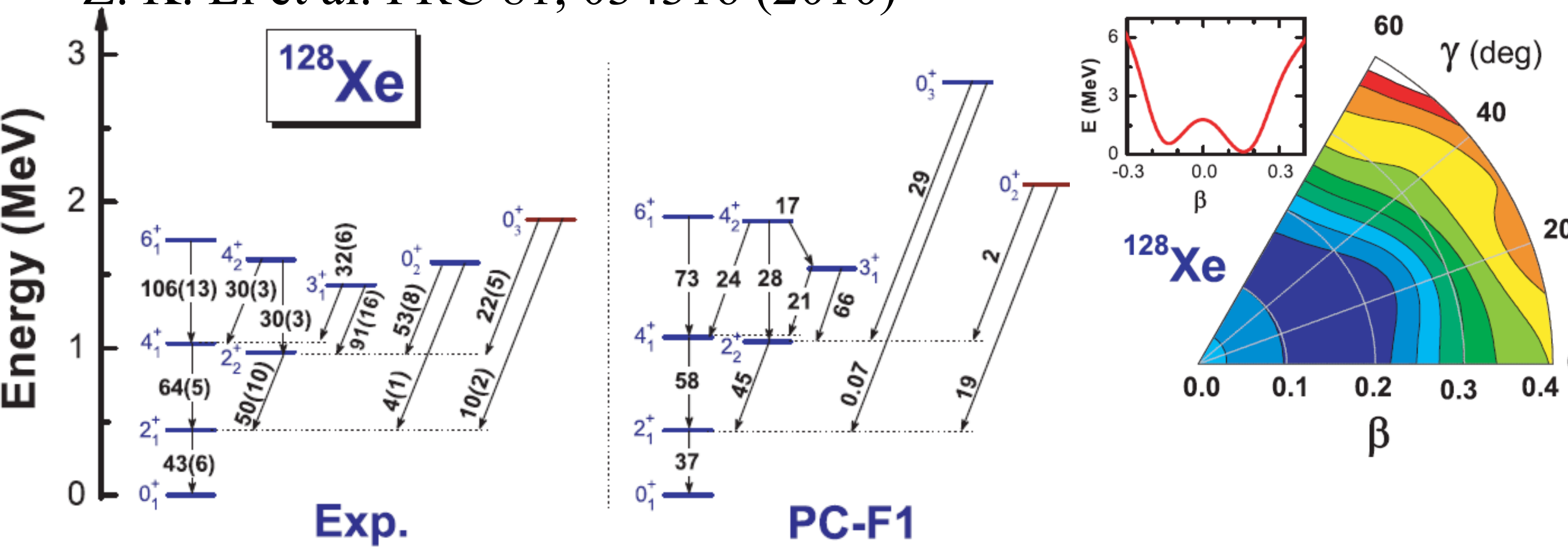
Spacing of the sp. levels reflects effective mass $M^*/M \sim 0.7$

Microscopic Bohr Hamiltonian

RMF EDF PC-F1
+ BCS pairing with delta force
+Cranking mass parameters
Beijing-Zagreb collaboration

Selected regions
of transitional nuclei

Example:
Z. K. Li et al. PRC 81, 034316 (2010)



Theoretical spectrum scaled to experimental 2^+_1 state. Calculated energies too large.

Generator Coordinates (GCM)

Skyrme EDF Sly4
+zero range pairing (Lipkin-Nogami)
+Angular momentum projection (topGOA)
+Hill-Wheeler with 6 axial deformation points

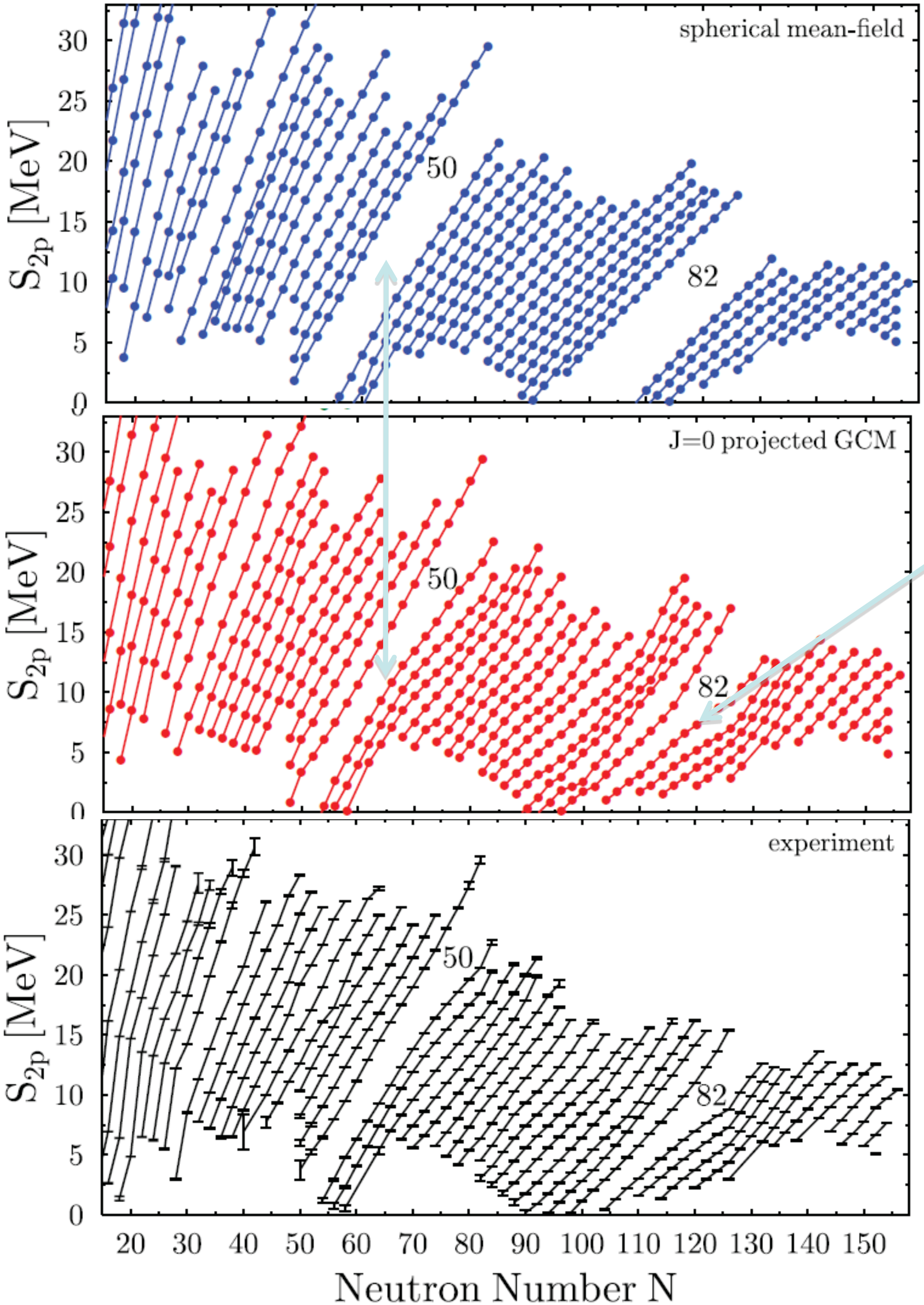
Bordeaux -Brussels – Seattle collaboration
Example:
M. Bender et al. PRC 78, 054312 (2008)

Theory	E	S_{2n}	S_{2p}	δ_{2n}	δ_{2p}	Q_α
Deformed SCMF	1.83	0.9	0.6	0.9	0.6	0.9
$+J=0$	1.70	0.8	0.5	0.7	0.5	0.8
+GCM	1.72	0.7	0.5	0.5	0.4	0.7

Improved binding energies

RMSDeviations from experiment

Energies of the 2^+_1 states far too large. Well known deficiency.

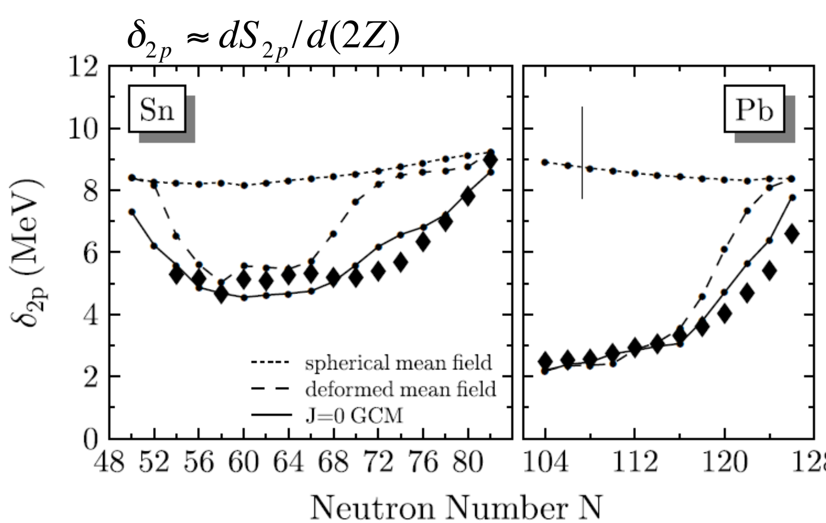


Effects of the
Quadrupole correlations

Reduction of the shell gaps

Quenching of the
Z=82 shell

Smoothes the rapid change
of $S_{2p/2n}$ near closed shells



Dipole strength function for deformed nuclei

Giant Resonances

Skyrme EDF, PC - RMF EDF,
FR - RMF, Gogny interaction

↓ consistent

QCD based

mean field +
residual interaction

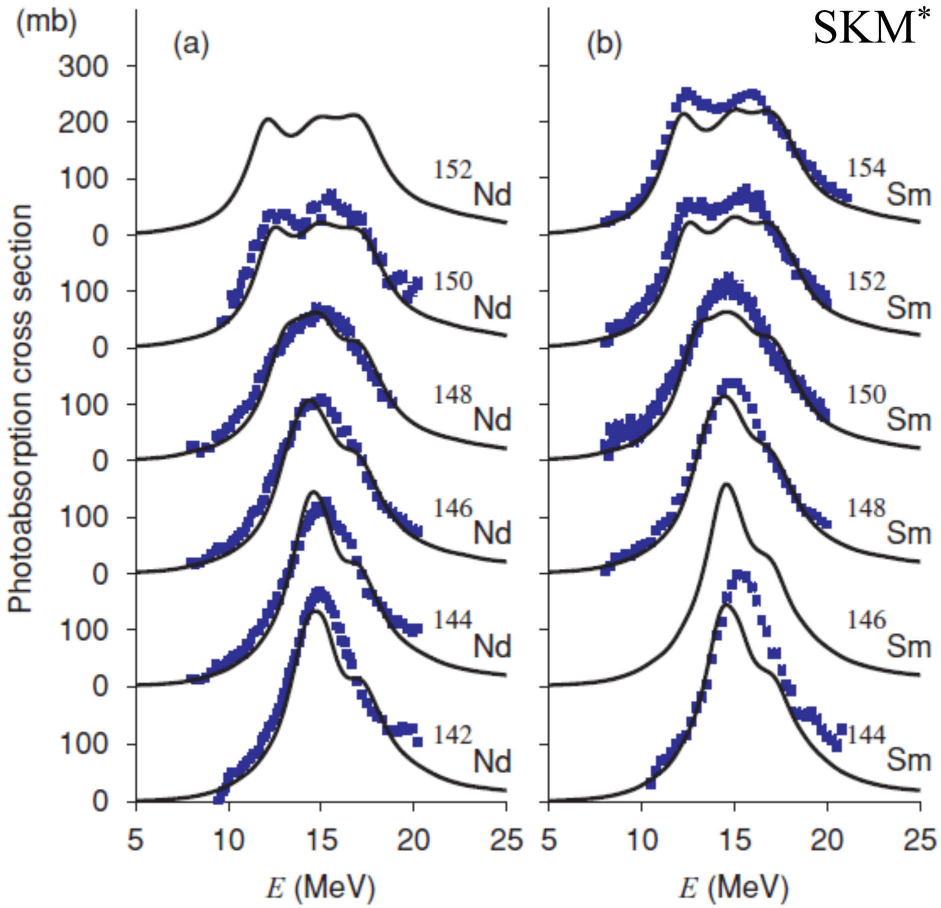
↓ Standard RPA: no problem for spherical nuclei

enormous numerical effort for heavy deformed nuclei

Strength functions:
E1, M1, GT, ...

Yoshida, Nakatsukasa PHYSICAL REVIEW C **83**, 021304(R) (2011)

500 h CPU/point
50% RPA matrix
50% digonalization
500 parallel CPU's



J. Terasaki and J. Engel, Phys. Rev. C 82, 034326 (2010): ^{172}Yb, SKP

Separable interactions derived from EDF

Based on understanding the physics,

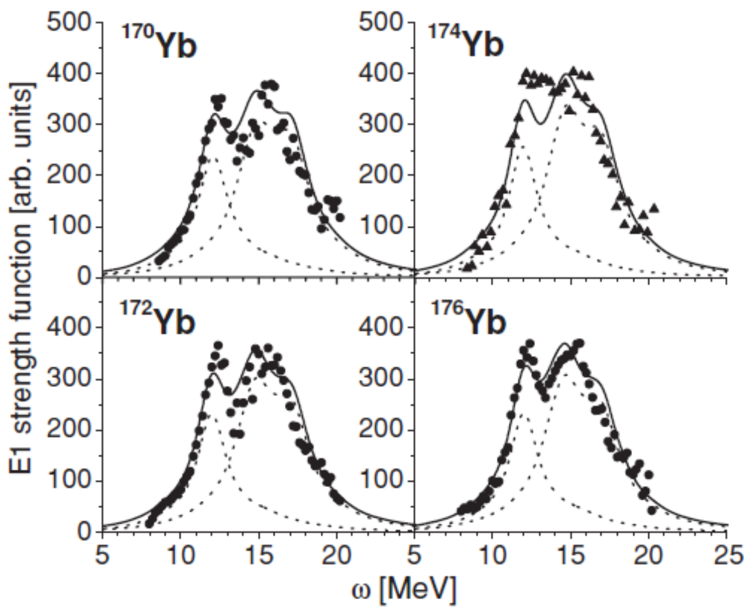
Guess few terms that describe the mode.

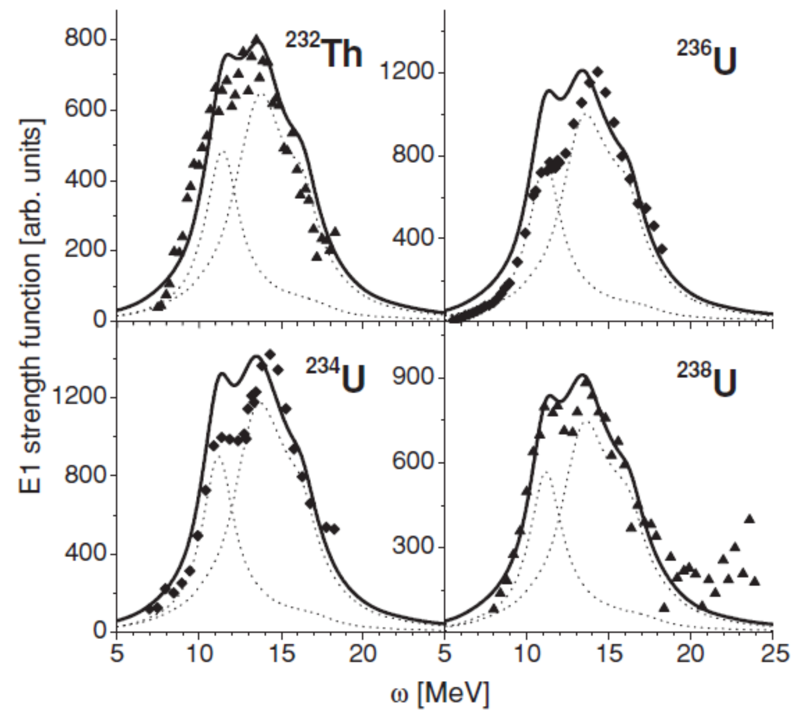
The coupling strength is derived from the EDF

You may miss important degrees of freedom!

Dubna-Erlangen-Prague collaboration

Kleinig et al. PHYSICAL REVIEW C **78, 044313 (2008)**





Fast enough for systematic calculation across the nuclear chart

RPA linearized periodic solution of TDHF

standard

Solution by
numerical diagonalization (250 CPU)
of a big hermitian matrix (250 CPU)

Direct numerical solution of the linear TDHF equations by iteration
Evaluation of each step by existing mean field code

computational scale ~ $(\text{sp. dim.})^2$

computational scale ~ $(\text{sp. dim.})^1$

Arnoldi iteration: solution in the harmonic oscillatior basis
Jyvaskylae-Warsaw group
J. Toivanen et al. PHYSICAL REVIEW C **81, 034312 (2010)**

FAM: solution on a spatial grid
RIKEN-Tsukuba group
T. Inakura et. al, PHYSICAL REVIEW C **80, 044301 (2009)**

Proof of principle with light and Spherical heavy nuclei