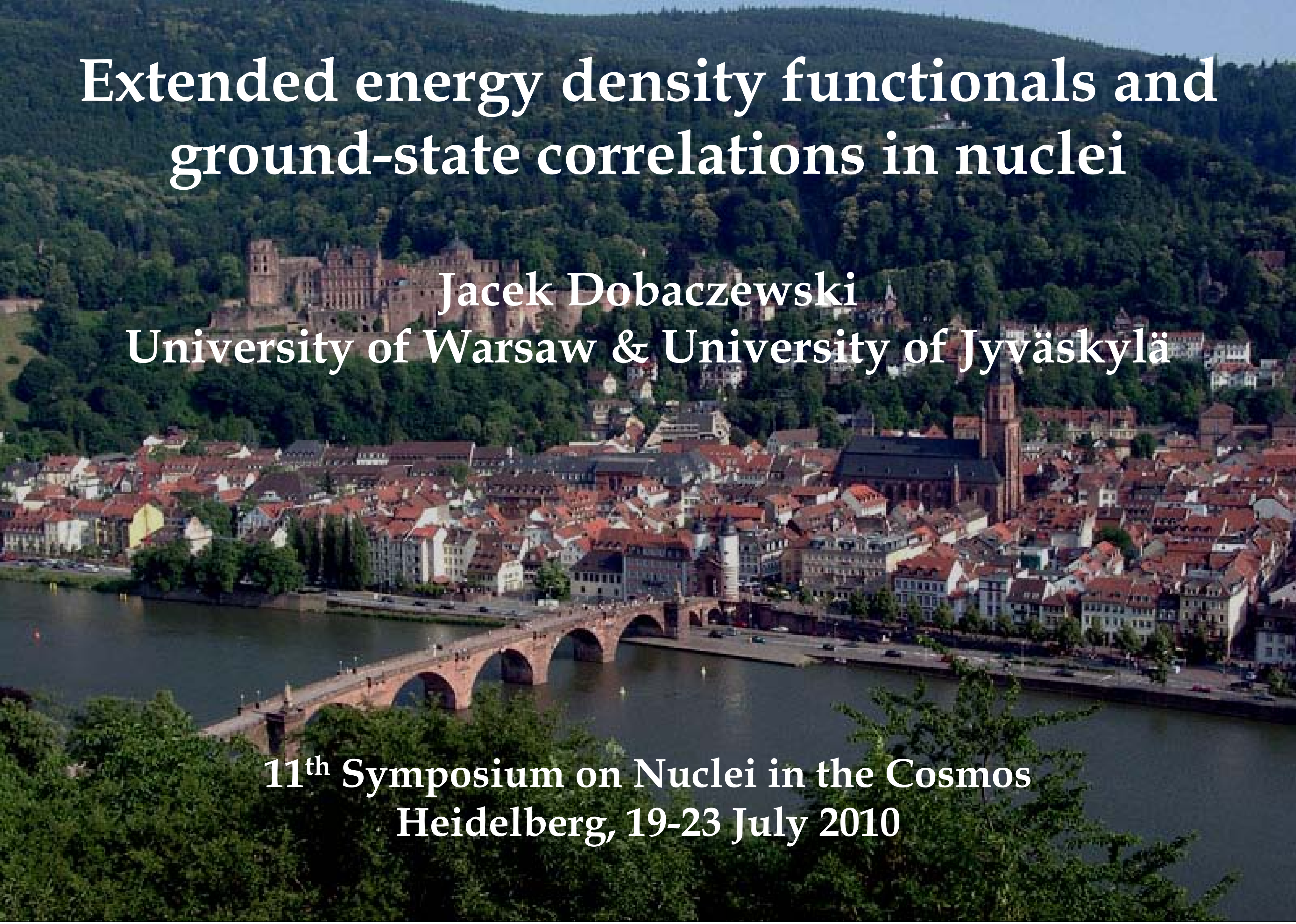
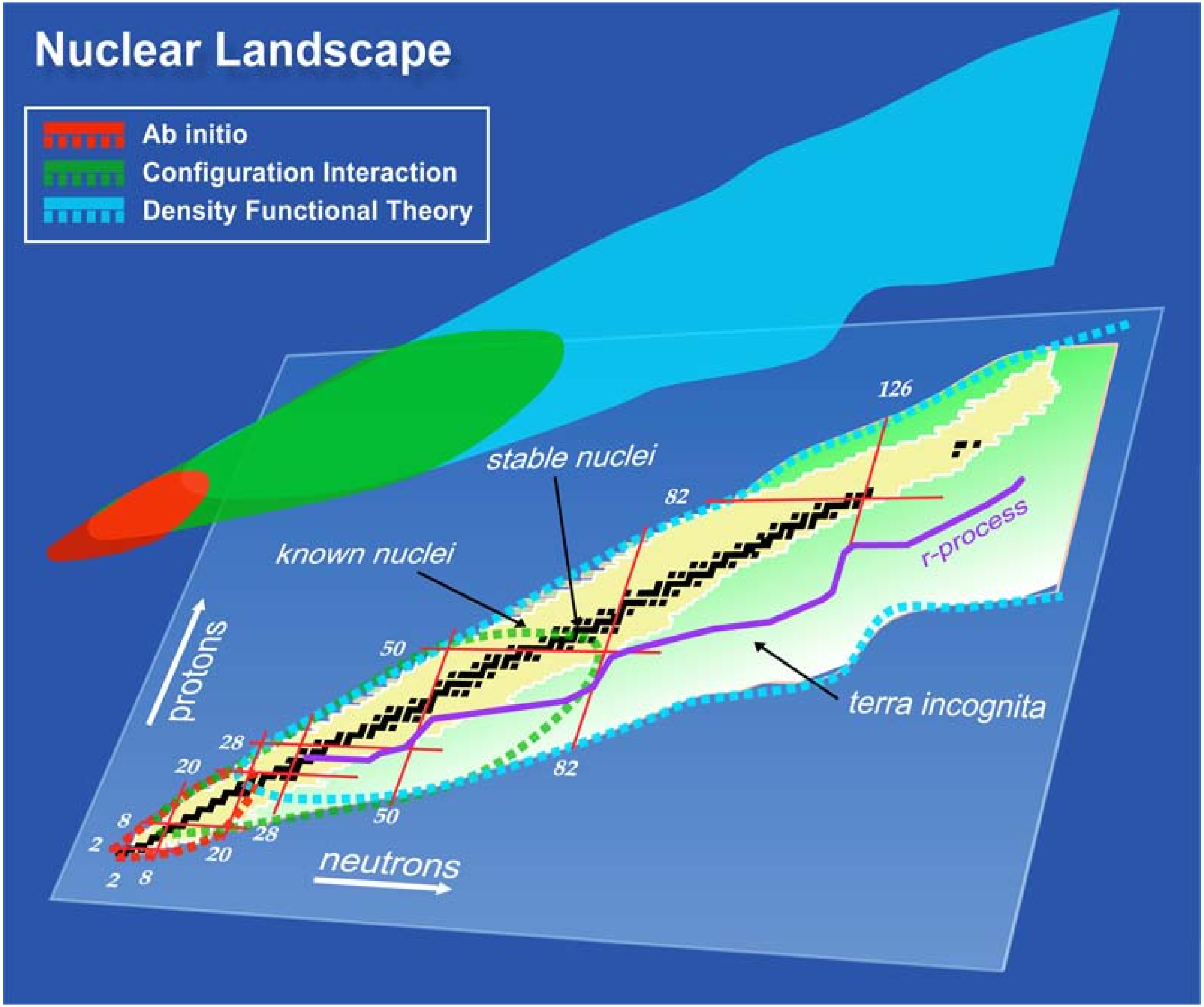


Extended energy density functionals and ground-state correlations in nuclei

Jacek Dobaczewski
University of Warsaw & University of Jyväskylä

11th Symposium on Nuclei in the Cosmos
Heidelberg, 19-23 July 2010

Universal Nuclear Energy Density Functional



UNEDF Collaboration, http://unedf.org/

What is DFT?

Density Functional Theory:

A variational method that uses observables as variational parameters.

$$\delta\langle\hat{H} - \lambda\hat{Q}\rangle = 0$$

$$\Downarrow$$

$$E = E(Q)$$

$$\text{for} \quad E(\lambda) \equiv \langle\hat{H}\rangle \qquad \text{and} \qquad Q(\lambda) \equiv \langle\hat{Q}\rangle$$

Which DFT?

$$\delta\langle\hat{H}-\lambda\hat{Q}\rangle=0 \Longrightarrow E=E(Q)$$

$$\delta\langle\hat{H}-\sum_k\lambda_k\hat{Q}_k\rangle=0 \Longrightarrow E=E(Q_k)$$

$$\delta\langle\hat{H}-\int\mathrm{d}q\,\lambda(q)\hat{Q}(q)\rangle=0 \Longrightarrow E=E[Q(q)]$$

$$\delta\langle\hat{H}-\int\mathrm{d}\vec{r}\,\lambda(\vec{r})\hat{\rho}(\vec{r})\rangle=0 \Longrightarrow E=E[\rho(\vec{r})]$$

$$\text{for}\quad \hat{\rho}(\vec{r}) \;=\; \sum_{i=1}^{A}\delta(\vec{r}-\vec{r}_i)$$

$$\delta\langle\hat{H}-\int\int\mathrm{d}\vec{r}\mathrm{d}\vec{r}\,'\,\lambda(\vec{r},\vec{r}\,')\hat{\rho}(\vec{r},\vec{r}\,')\rangle=0 \Longrightarrow E=E[\rho(\vec{r},\vec{r}\,')]$$

What is the DFT good for?

$$\delta\langle\hat{H} - \lambda\hat{Q}\rangle = 0$$
$$\Downarrow$$
$$E = E(Q)$$

Energy E is a function(al) of Q

1) **Exact:** Minimization of E(Q) gives the exact E and exact Q
2) **Impractical:** Derivation of E(Q) requires the full variation δ (bigger effort than to find the exact ground state)
3) **Inspirational:** Can we build useful models E′(Q) of the exact E(Q)?
4) **Experiment-driven:** E′(Q) works better or worse depending on the physical input used to build it.

Nuclear Energy Density Functionals

How the nuclear EDF is built?

Non-local energy density is a function of non-local density

$$E'[\rho(\vec{r},\vec{r}\,')] = \iint \mathrm{d}\vec{r}\,\mathrm{d}\vec{r}\,'\,\mathcal{H}(\rho(\vec{r},\vec{r}\,'))$$

Gogny, M3Y,...

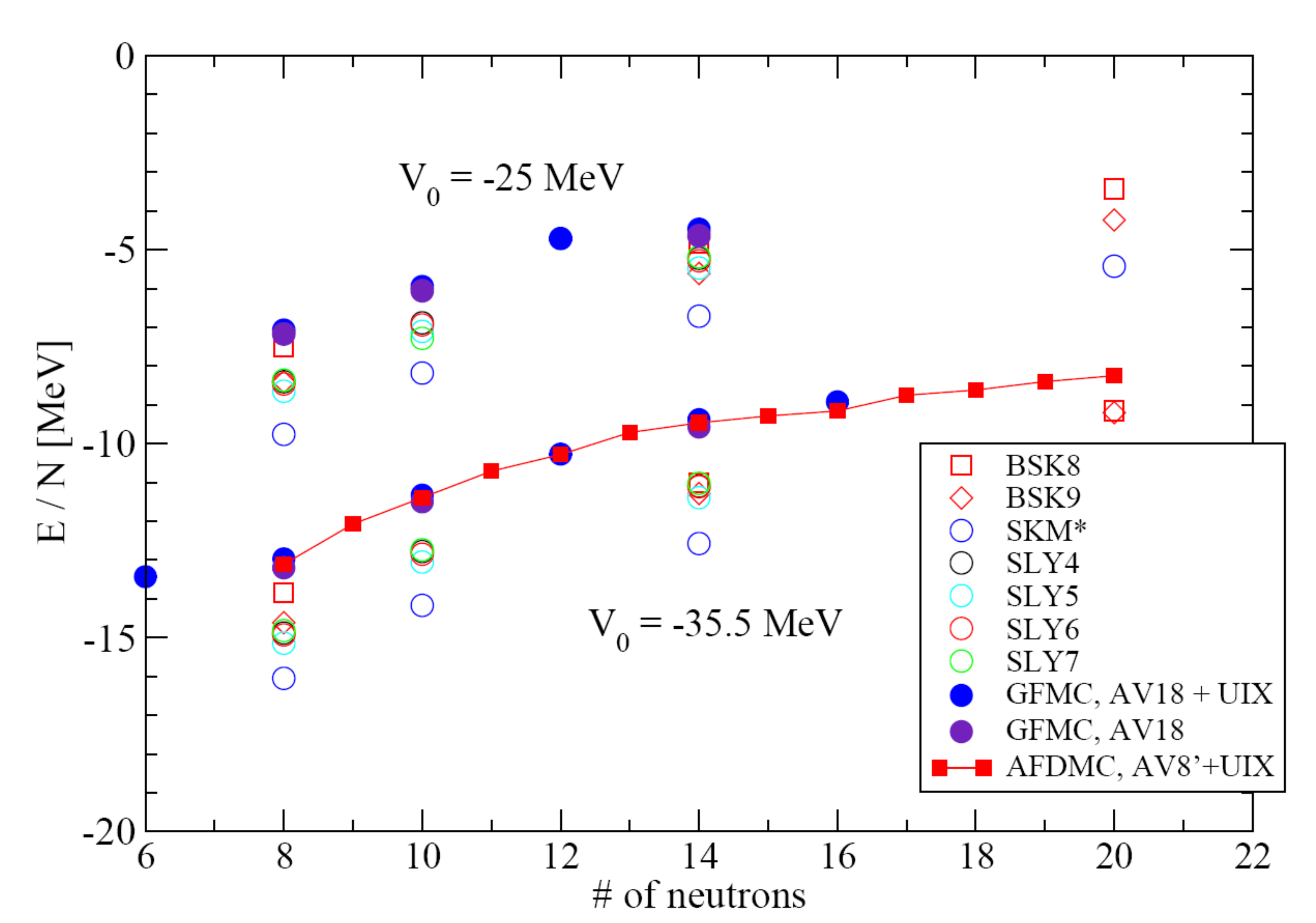
$$\mathcal{H}(\rho(\vec{r},\vec{r}\,')) = V(\vec{r}-\vec{r}\,')\Big[\rho(\vec{r})\rho(\vec{r}\,') - \rho(\vec{r},\vec{r}\,')\rho(\vec{r}\,',\vec{r})\Big]$$

Quasi-local energy density is a function of local densities and gradients

$$E' = \int \mathrm{d}\vec{r}\,\mathcal{H}(\rho(\vec{r}),\tau(\vec{r}),\Delta\rho(\vec{r}),\ldots)$$

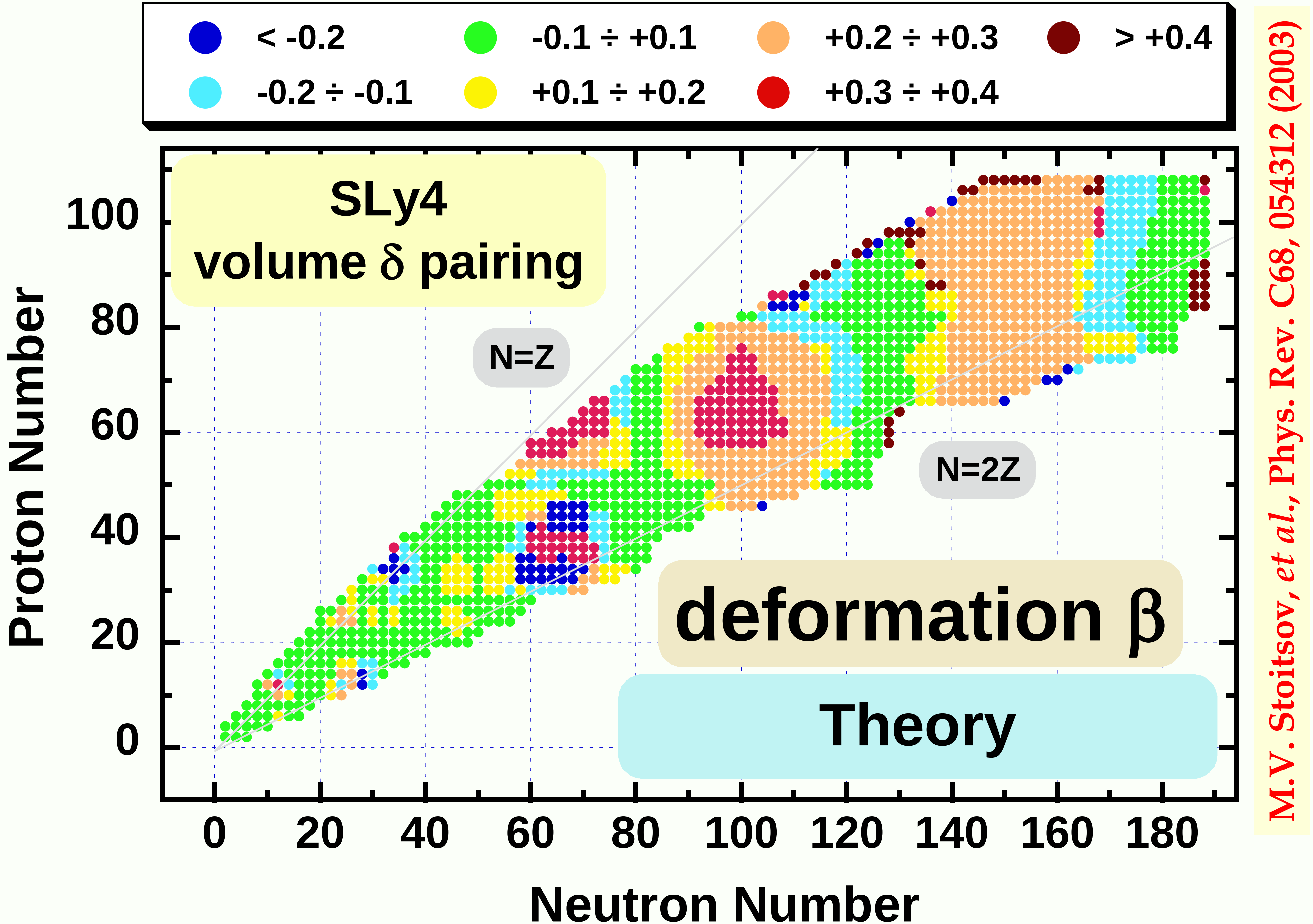
Skyrme, BCP, point-coupling,...

Neutrons in external Woods-Saxon well

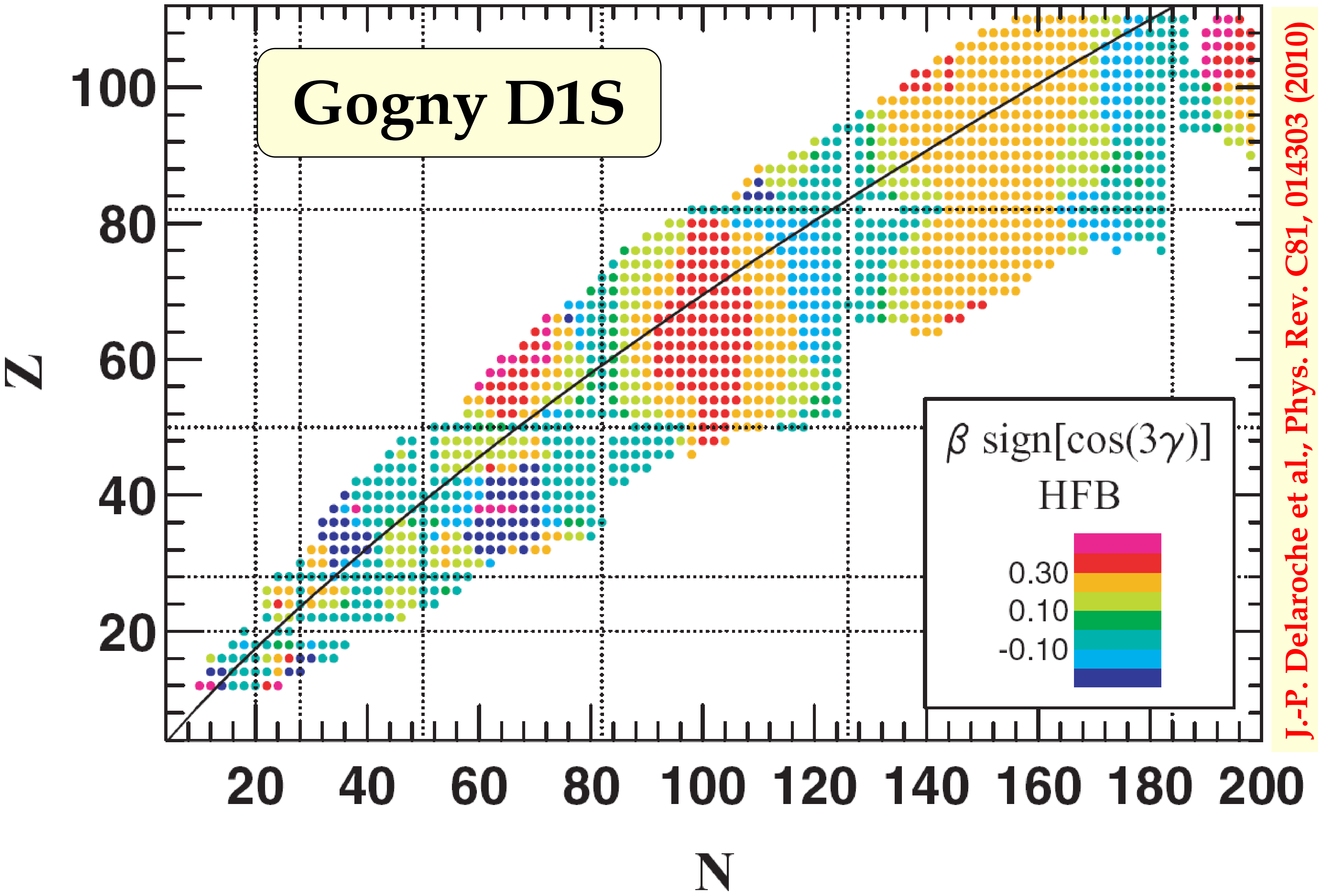


R.B. Wiringa & UNEDF Collaboration

Applications

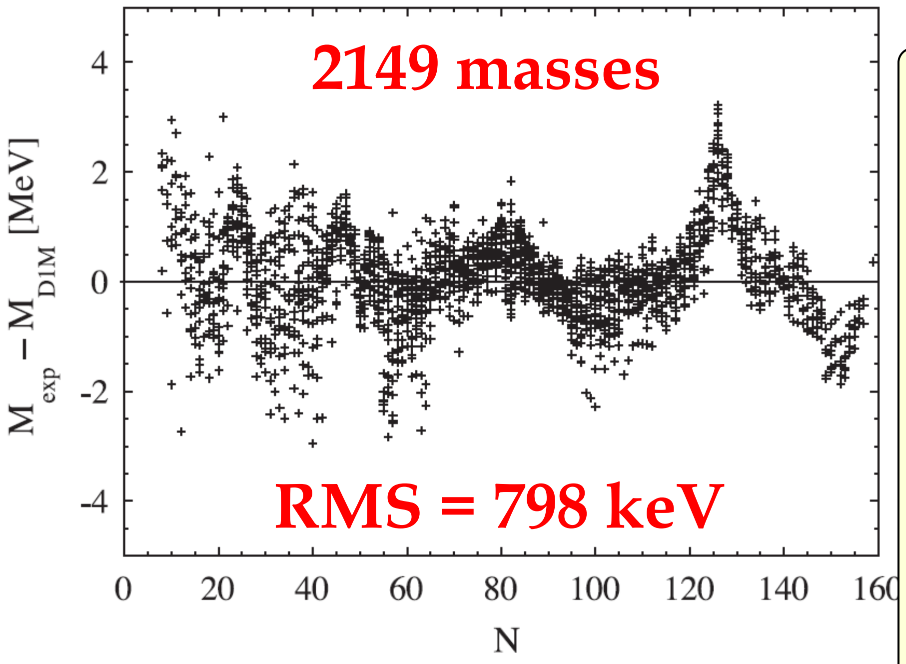


< -0.2
-0.1 ÷ +0.1
+0.2 ÷ +0.3
> +0.4
-0.2 ÷ -0.1
+0.1 ÷ +0.2
+0.3 ÷ +0.4
SLy4
volume δ pairing
N=Z
N=2Z
deformation β
Theory
Proton Number
Neutron Number
0
20
40
60
80
100
120
140
160
180
M.V. Stoitsov, et al., Phys. Rev. C68, 054312 (2003)



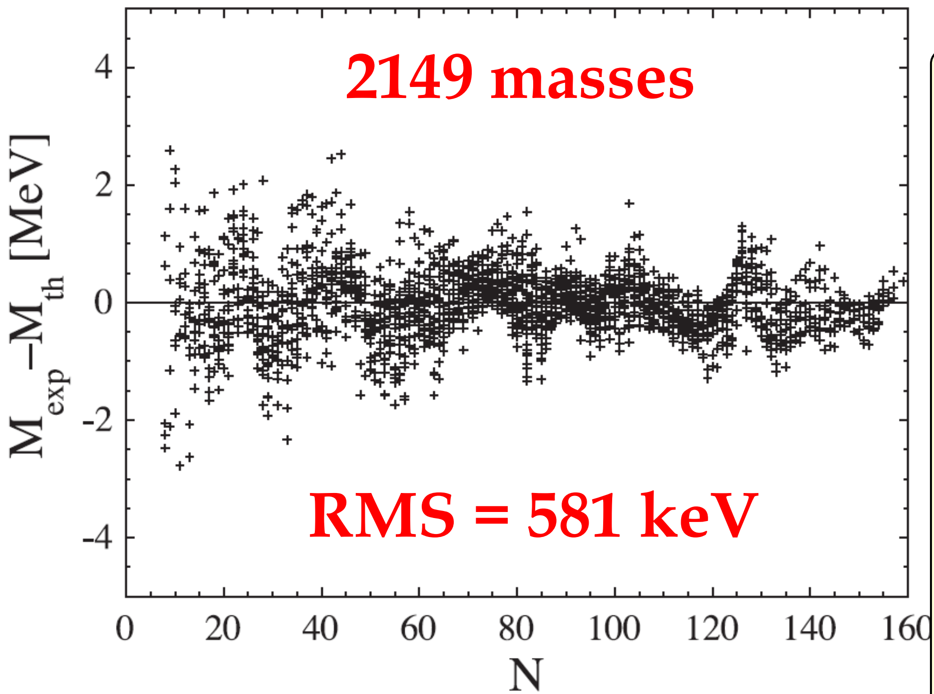
J.-P. Delaroche et al., Phys. Rev. C81, 014303 (2010)

Nuclear binding energies (masses)



S. Goriely *et al.*, Phys. Rev. Lett. 102, 242501 (2009)

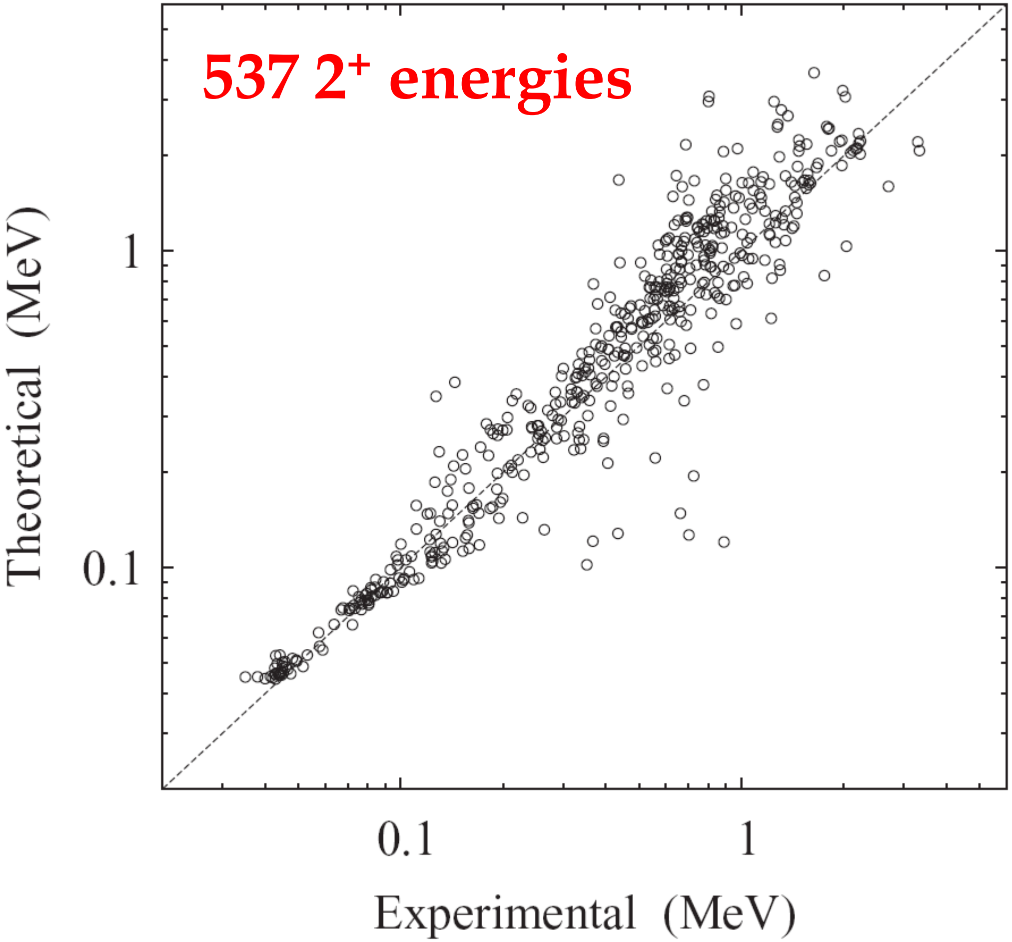
The first Gogny HFB mass model. An explicit and self-consistent account of all the quadrupole correlation energies are included within the 5D collective Hamiltonian approach.



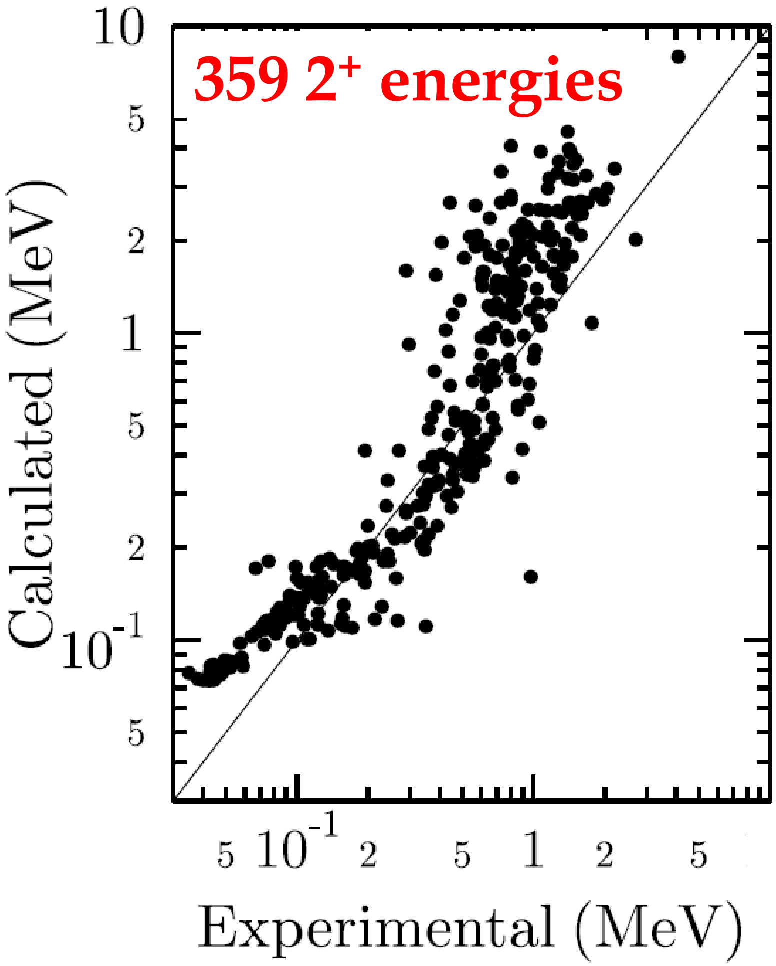
S. Goriely *et al.*, Phys. Rev. Lett. 102, 152503 (2009)

The new Skyrme HFB nuclear-mass model, in which the contact-pairing force is constructed from microscopic pairing gaps of symmetric nuclear matter and neutron matter.

First 2^+ excitations of even-even nuclei



J.-P. Delaroche *et al.*, Phys. Rev. C81, 014303 (2010)

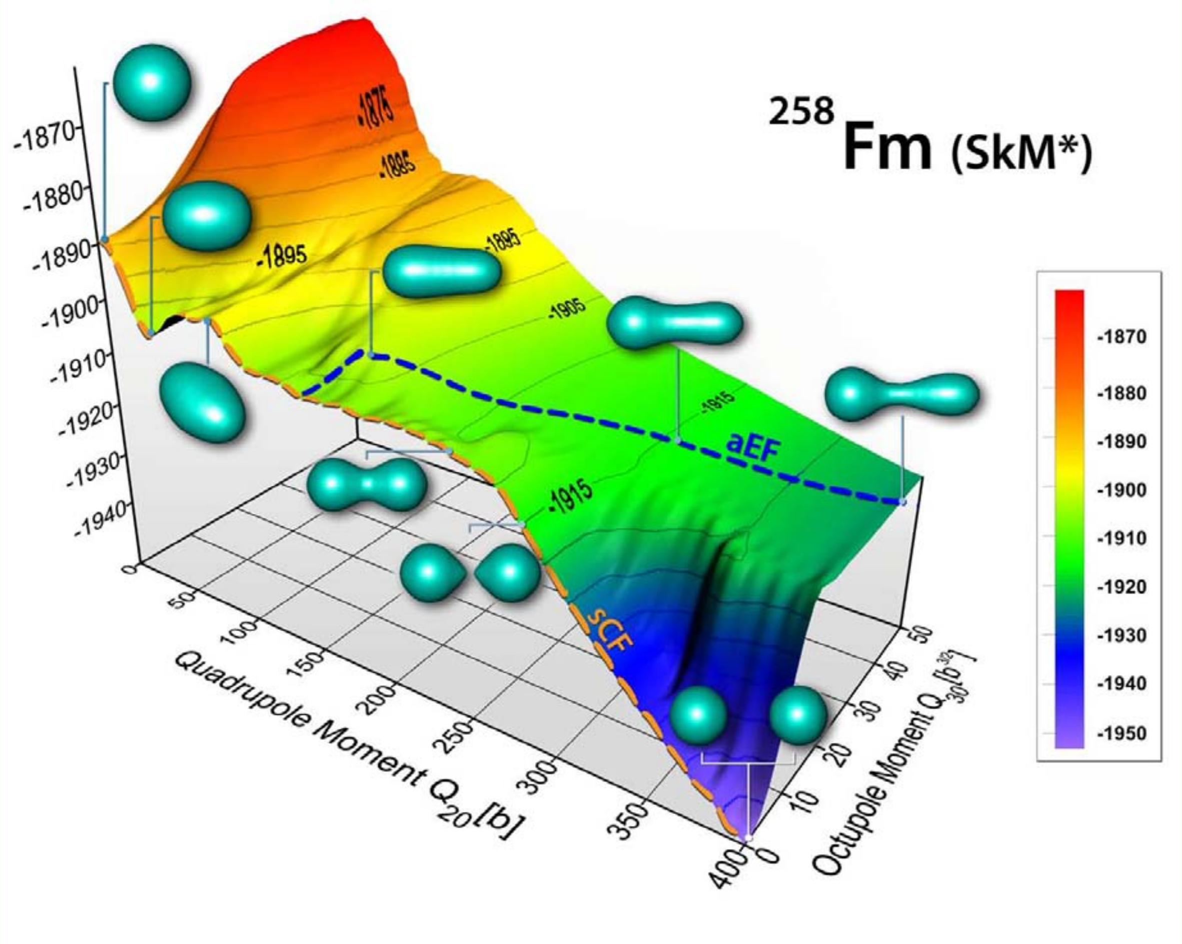


B. Sabbey *et al.*, Phys. Rev. C75, 044305 (2007)

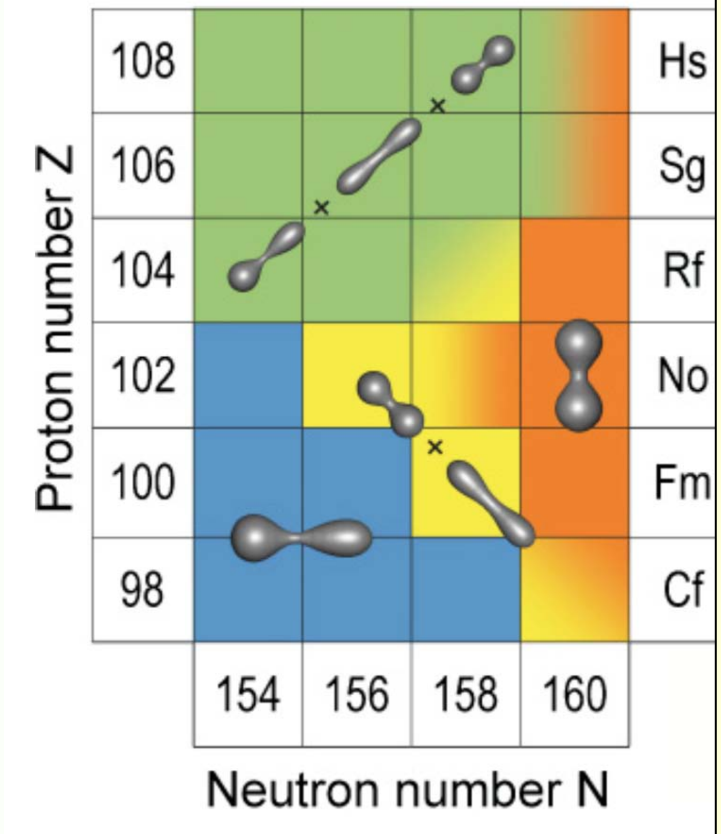
Gogny HFB calculations plus the 5D collective Hamiltonian approach.

Skyrme HF+BCS calculations plus the particle-number and angular-momentum projection and shape mixing.

Spontaneous fission



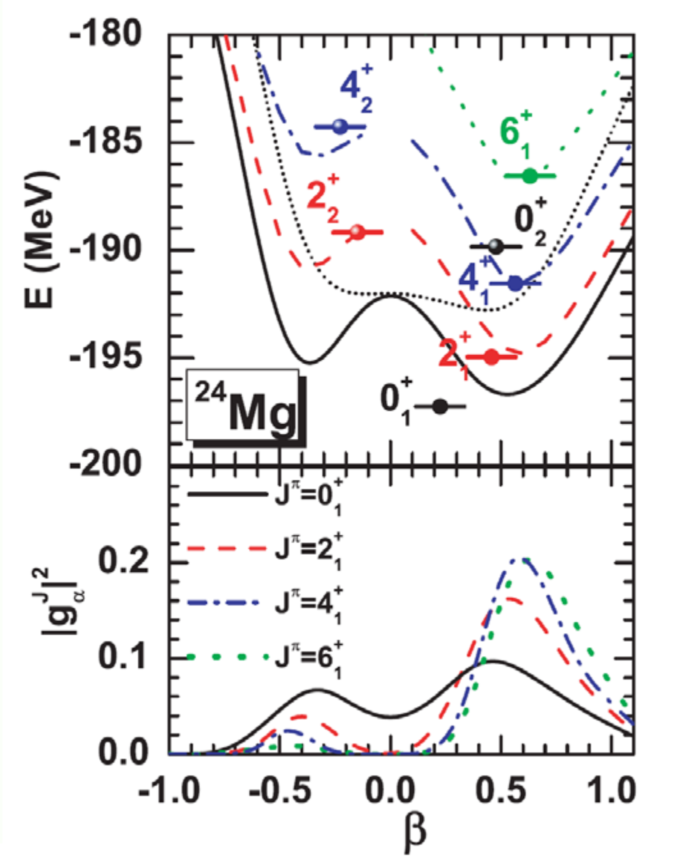
UNEDF collaboration: SciDAC Review 6, 42 (2007)

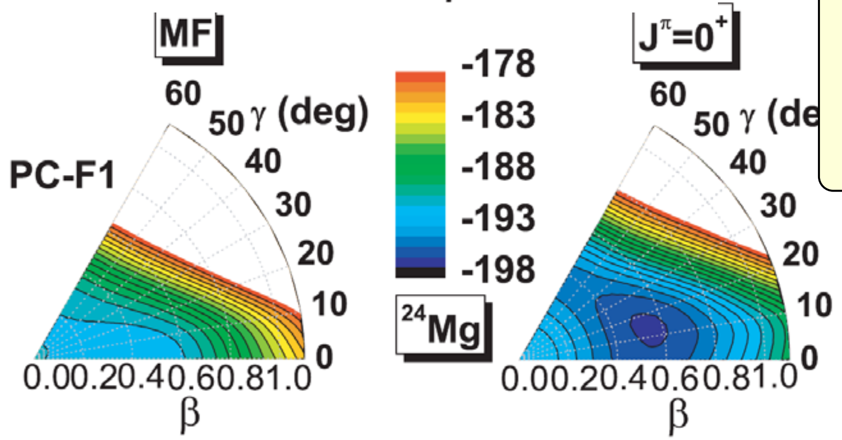


A. Staszczak *et al.*, Phys. Rev. C80, 014309 (2009)

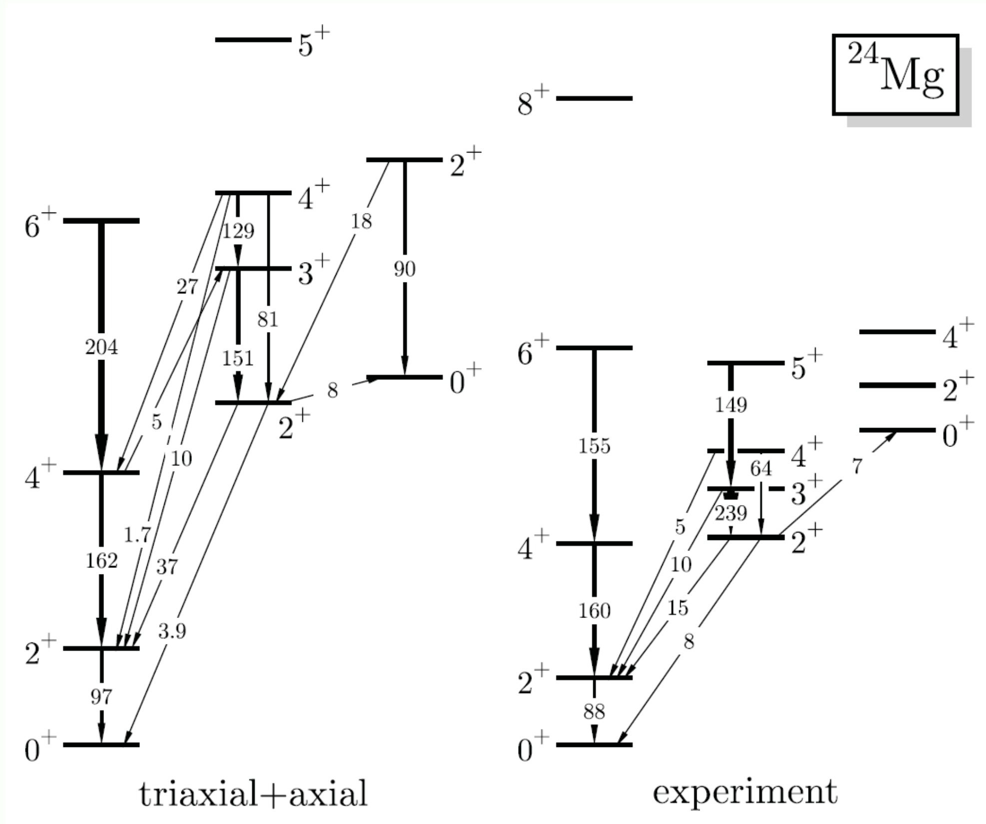
Symmetry-unrestricted Skyrme HF+BCS calculations.

Collective states in even-even nuclei





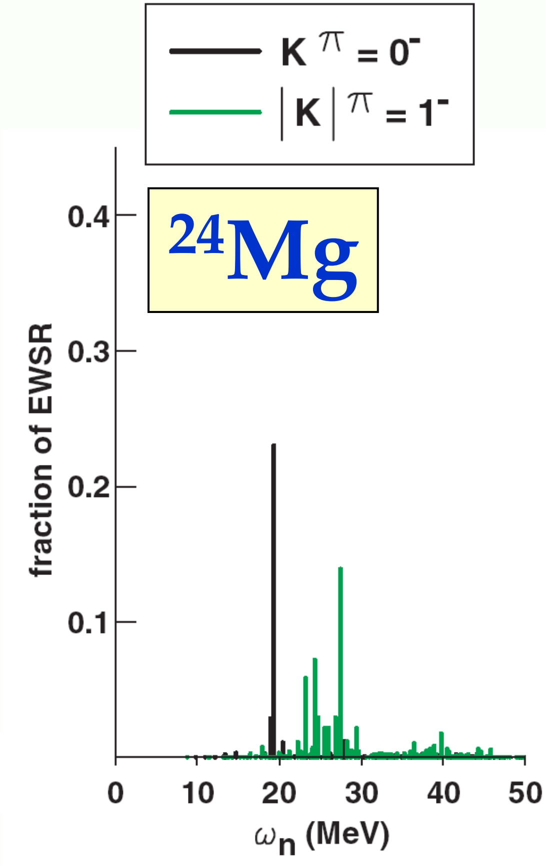
J.M. Yao *et al.*, Phys. Rev. C81, 044311 (2010)



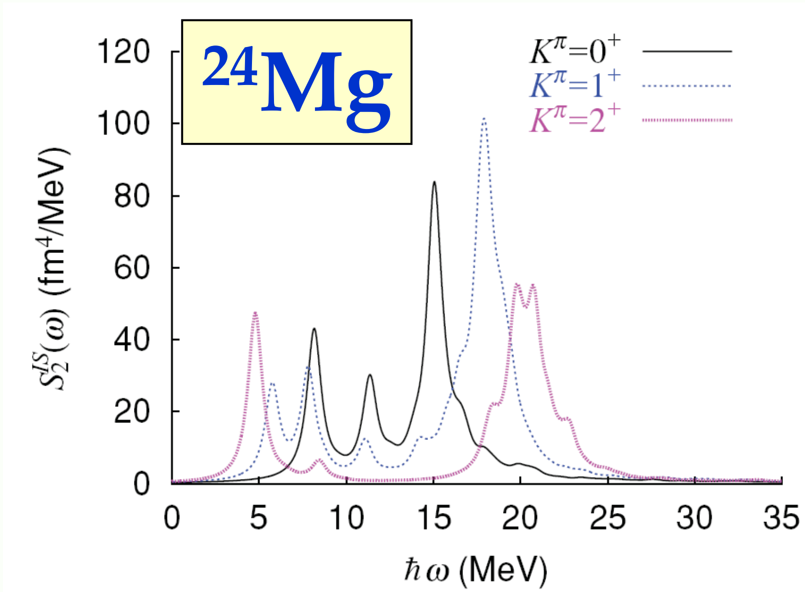
M. Bender *et al.*, Phys. Rev. C78, 024309 (2008)

$$|\Psi_{NZ,JM}\rangle = \int \mathrm{d}\beta \mathrm{d}\gamma \sum_K f_K(\beta,\gamma) \times \hat{P}_N \hat{P}_Z \hat{P}_{JMK} |\Psi(\beta,\gamma)\rangle$$

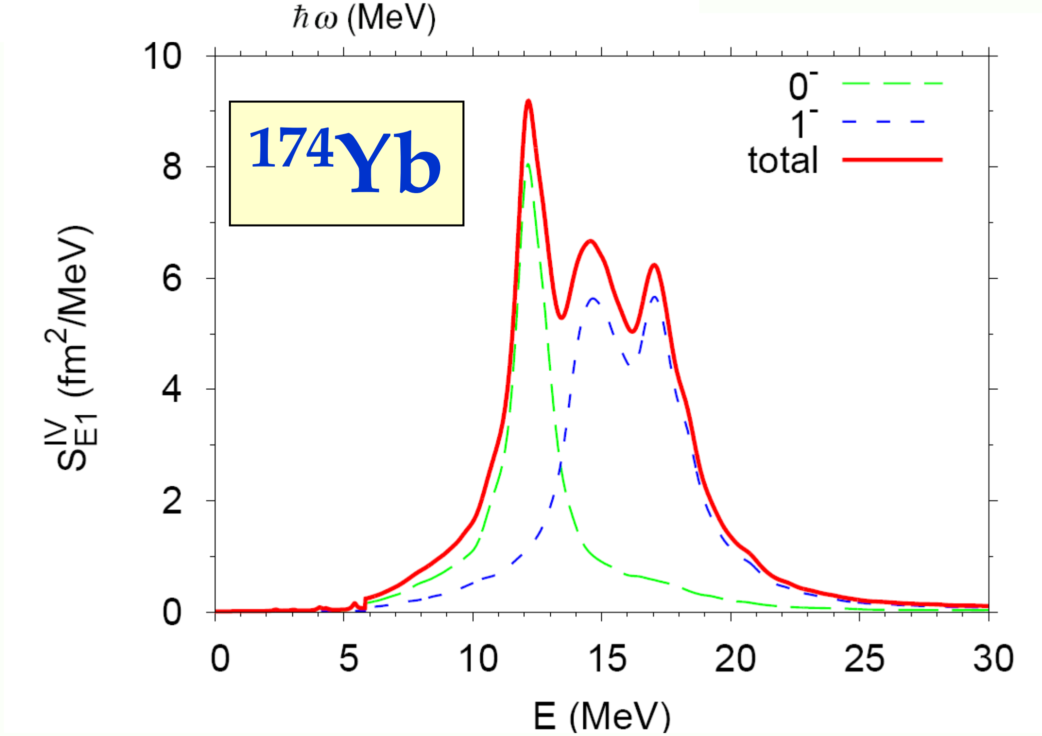
Giant resonances in deformed nuclei



S. Péru *et al.*, Phys. Rev. C77, 044313 (2008)



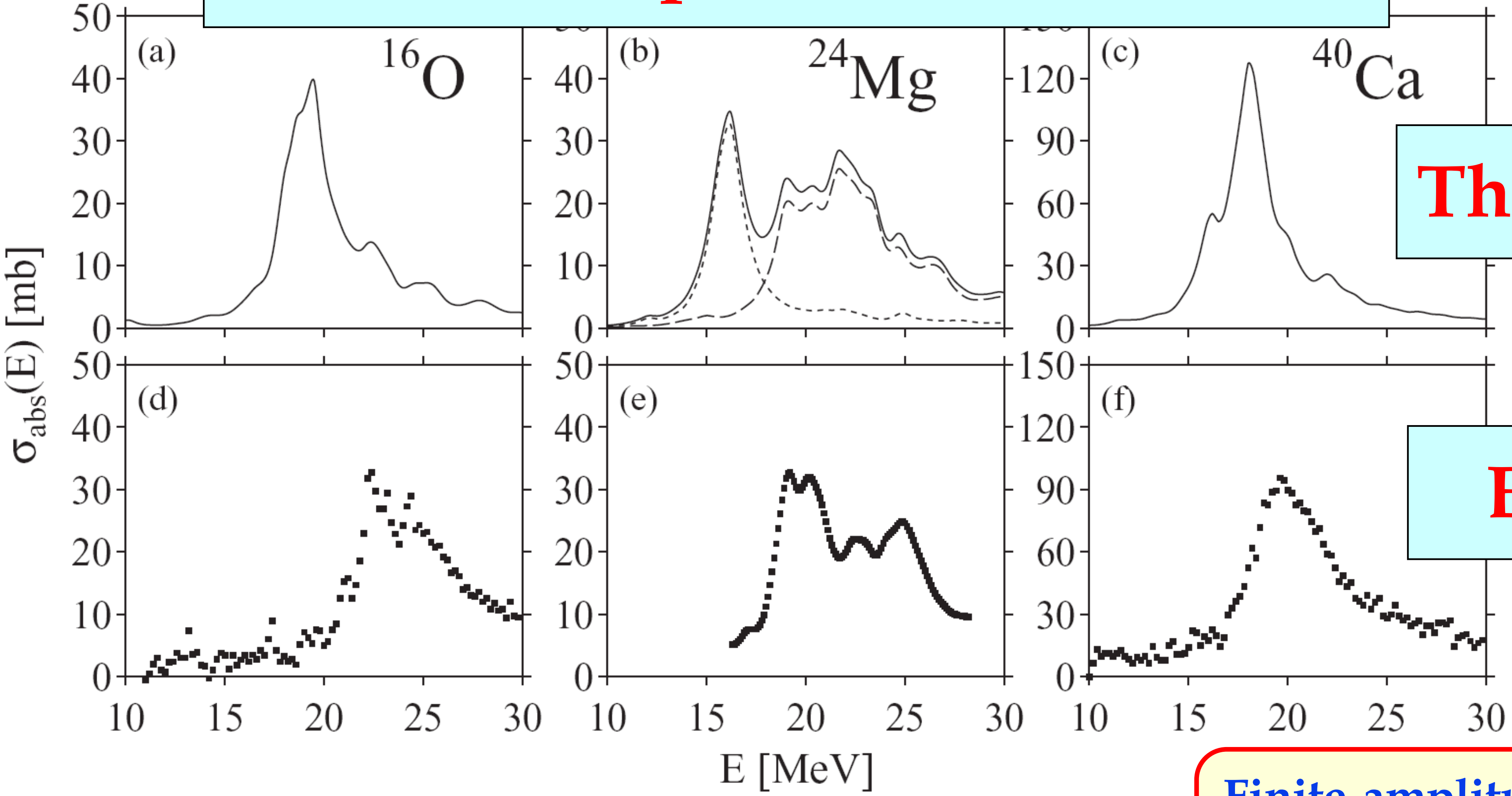
K. Yoshida *et al.*, Phys. Rev. C78, 064316 (2008)



J. Terasaki *et al.*, arXiv:1006.0010

Iterative methods to solve (Q)RPA

Photoabsorption cross sections



Theory

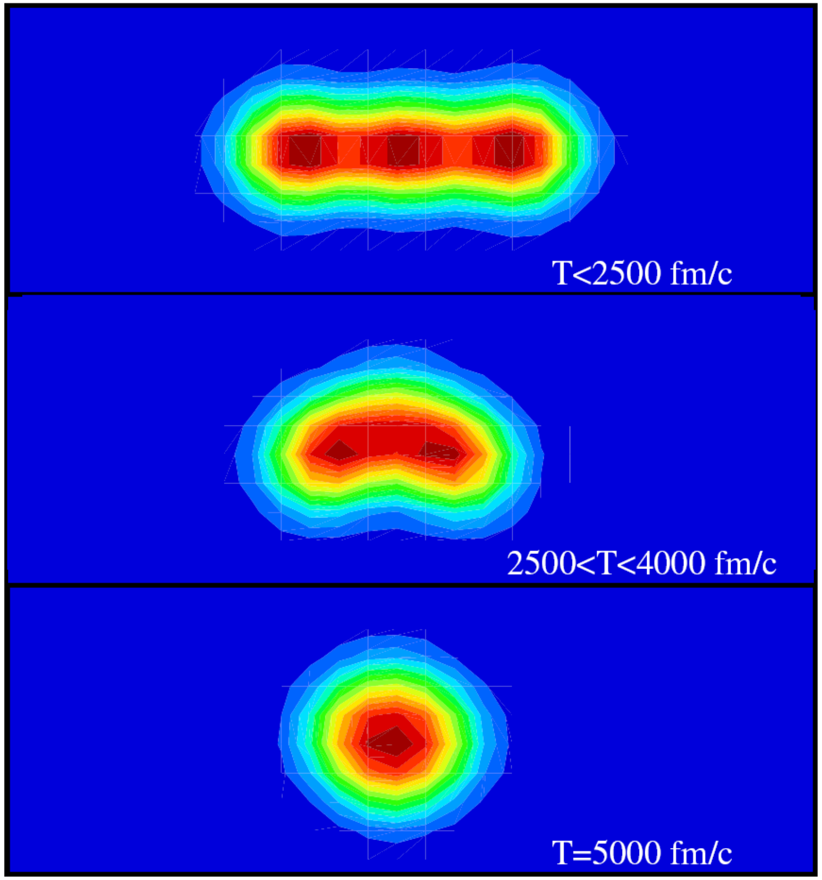
Exp

T. Inakura *et al.*, Phys. Rev. C80, 044301 (2009)

Finite-amplitude method to solve the QRPA equations.

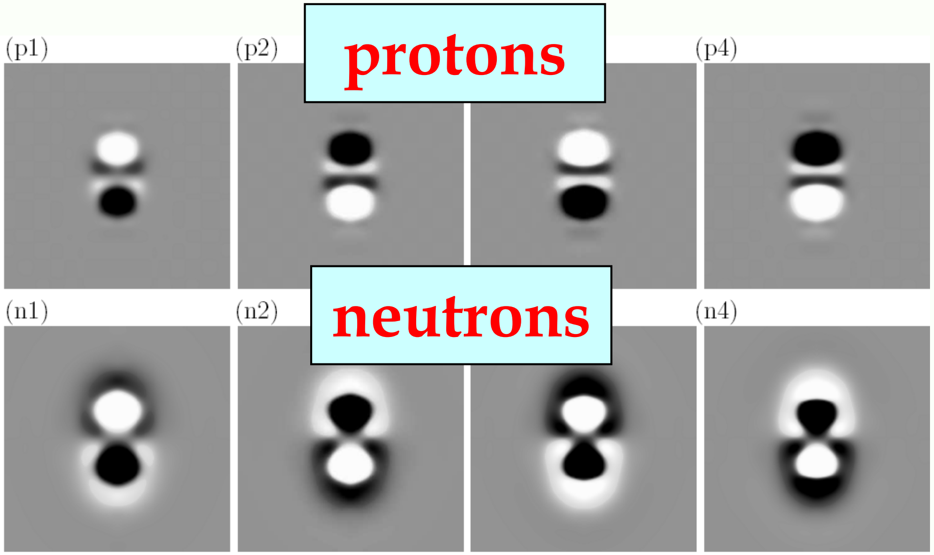
Time-dependent solutions

α– ^{8}Be collision (tip configuration)



A.S. Umar *et al.*, Phys. Rev. Lett. 104, 212503 (2010)

Dipole oscillations in ^{14}Be



T. Nakatsukasa *et al.*, Nucl. Phys. A788, 349 (2007)

UNEDF collaboration: Quantum Dynamics with TDSLDA, A. Bulgac, *et al.*, http://www.phys.washington.edu/groups/qmbnt/index.html

Nuclear Energy Density Functional

We consider the EDF in the form,

$$\mathcal{E} = \int d^3r \mathcal{H}(r),$$

where the energy density $\mathcal{H}(r)$ can be represented as a sum of the kinetic energy and of the potential-energy isoscalar ($t = 0$) and isovector ($t = 1$) terms,

$$\mathcal{H}(r) = \frac{\hbar^2}{2m}\tau_0 + \mathcal{H}_0(r) + \mathcal{H}_1(r),$$

which for the time-reversal and spherical symmetries imposed read:

$$\mathcal{H}_t(r) = C_t^\rho \rho_t^2 + C_t^\tau \rho_t \tau_t + C_t^{\Delta\rho} \rho_t \Delta\rho_t + \tfrac{1}{2} C_t^J J_t^2 + C_t^{\nabla J} \rho_t \nabla \cdot J_t.$$

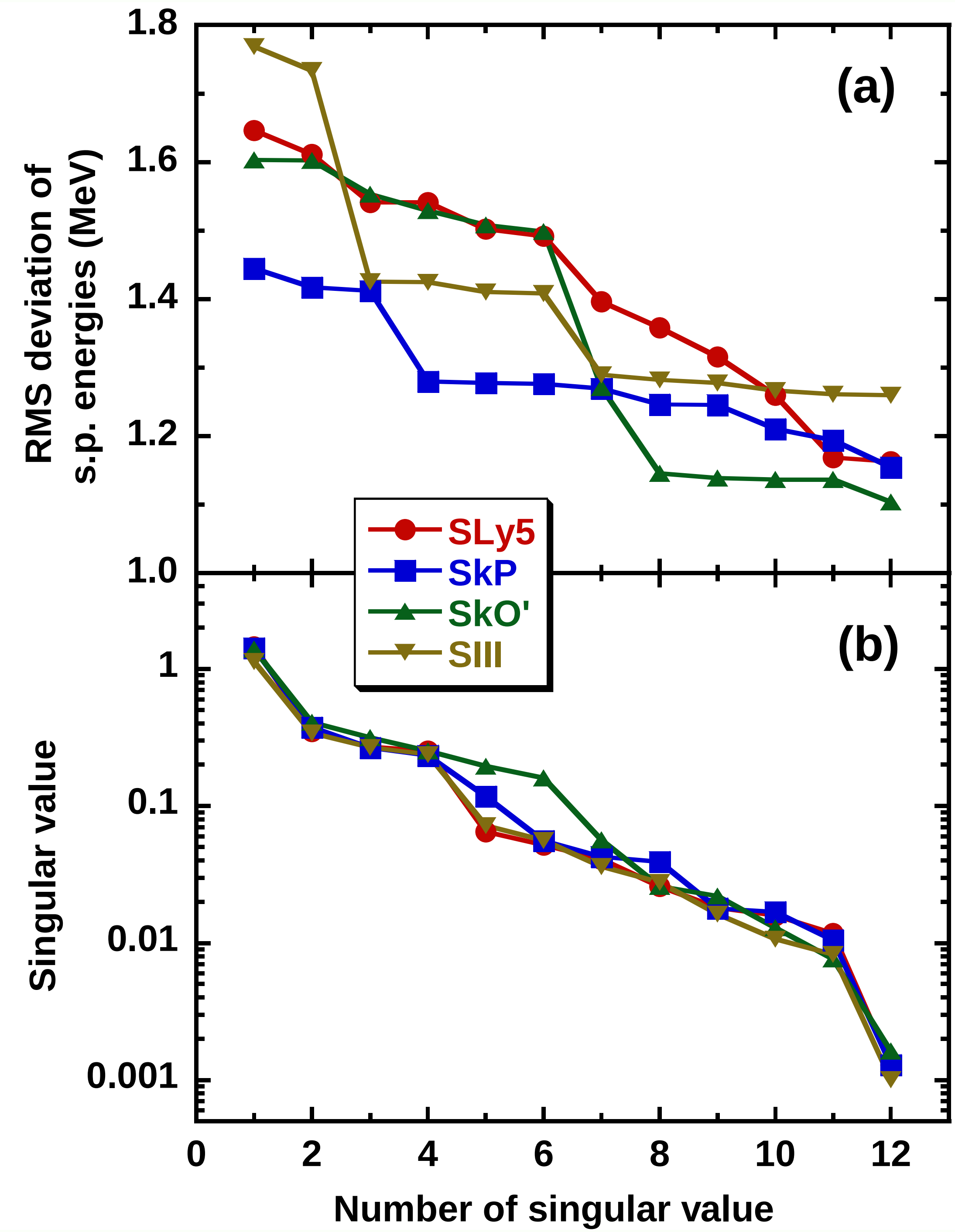
Following the parametrization used for the Skyrme forces, we assume the dependence of the coupling parameters C_t^ρ on the isoscalar density ρ_0 as:

$$C_t^\rho = C_{t0}^\rho + C_{t\mathrm{D}}^\rho \rho_0^\alpha.$$

The standard EDF depends linearly on 12 coupling constants,

$$C_{t0}^\rho, \quad C_{t\mathrm{D}}^\rho, \quad C_t^\tau, \quad C_t^{\Delta\rho}, \quad C_t^{\mathrm{J}}, \quad \text{and} \quad C_t^{\nabla \mathrm{J}},$$

for $t = 0$ and 1.



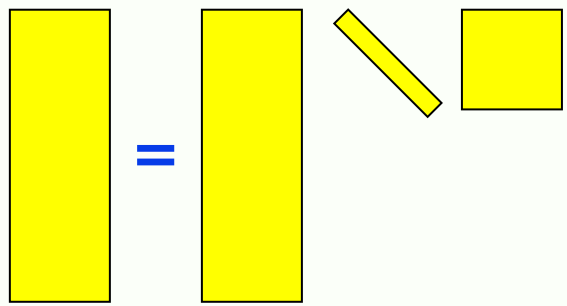
Fits of s.p. energies

$$\epsilon_i - \epsilon_i^{\mathrm{EXP}} = -\sum_m \beta_{im} \Delta C_m,$$

EXP: M.N. Schwierz, I. Wiedenhover, and A. Volya, arXiv:0709.3525

Singular value decomposition

$$\beta_{im} = \sum_\mu V_{i\mu} d_\mu U^T_{\mu m},$$



$$\sum_i V_{i\mu} V_{i\nu} = \delta_{\mu\nu},$$

$$\sum_m U_{m\mu} U_{m\nu} = \delta_{\mu\nu},$$

M. Kortelainen *et al.*, Phys. Rev. C77, 064307 (2008)

Derivatives of higher order: Negele & Vautherin density matrix expansion

Nr	Tensor	order n	rank L
1	1	0	0
2	∇	1	1
3	Δ	2	0
4	$[\nabla\nabla]_2$	2	2
5	$\Delta\nabla$	3	1
6	$[\nabla[\nabla\nabla]_2]_3$	3	3
7	Δ^2	4	0
8	$\Delta[\nabla\nabla]_2$	4	2
9	$[\nabla[\nabla[\nabla\nabla]_2]_3]_4$	4	4
10	$\Delta^2\nabla$	5	1
11	$\Delta[\nabla[\nabla\nabla]_2]_3$	5	3
12	$[\nabla[\nabla[\nabla[\nabla\nabla]_2]_3]_4]_5$	5	5
13	Δ^3	6	0
14	$\Delta^2[\nabla\nabla]_2$	6	2
15	$\Delta[\nabla[\nabla[\nabla\nabla]_2]_3]_4$	6	4
16	$[\nabla[\nabla[\nabla[\nabla[\nabla\nabla]_2]_3]_4]_5]_6$	6	6

Total derivatives $(\vec{\nabla}^m)_I$ up to N^{3}LO

Nr	Tensor	order n	rank L
1	1	0	0
2	k	1	1
3	k^2	2	0
4	$[kk]_2$	2	2
5	k^2k	3	1
6	$[k[kk]_2]_3$	3	3
7	$(k^2)^2$	4	0
8	$k^2[kk]_2$	4	2
9	$[k[k[kk]_2]_3]_4$	4	4
10	$(k^2)^2k$	5	1
11	$k^2[k[kk]_2]_3$	5	3
12	$[k[k[k[kk]_2]_3]_4]_5$	5	5
13	$(k^2)^3$	6	0
14	$(k^2)^2[kk]_2$	6	2
15	$k^2[k[k[kk]_2]_3]_4$	6	4
16	$[k[k[k[k[kk]_2]_3]_4]_5]_6$	6	6

Relative derivatives $(\vec{k}^n)_L$ up to N^{3}LO

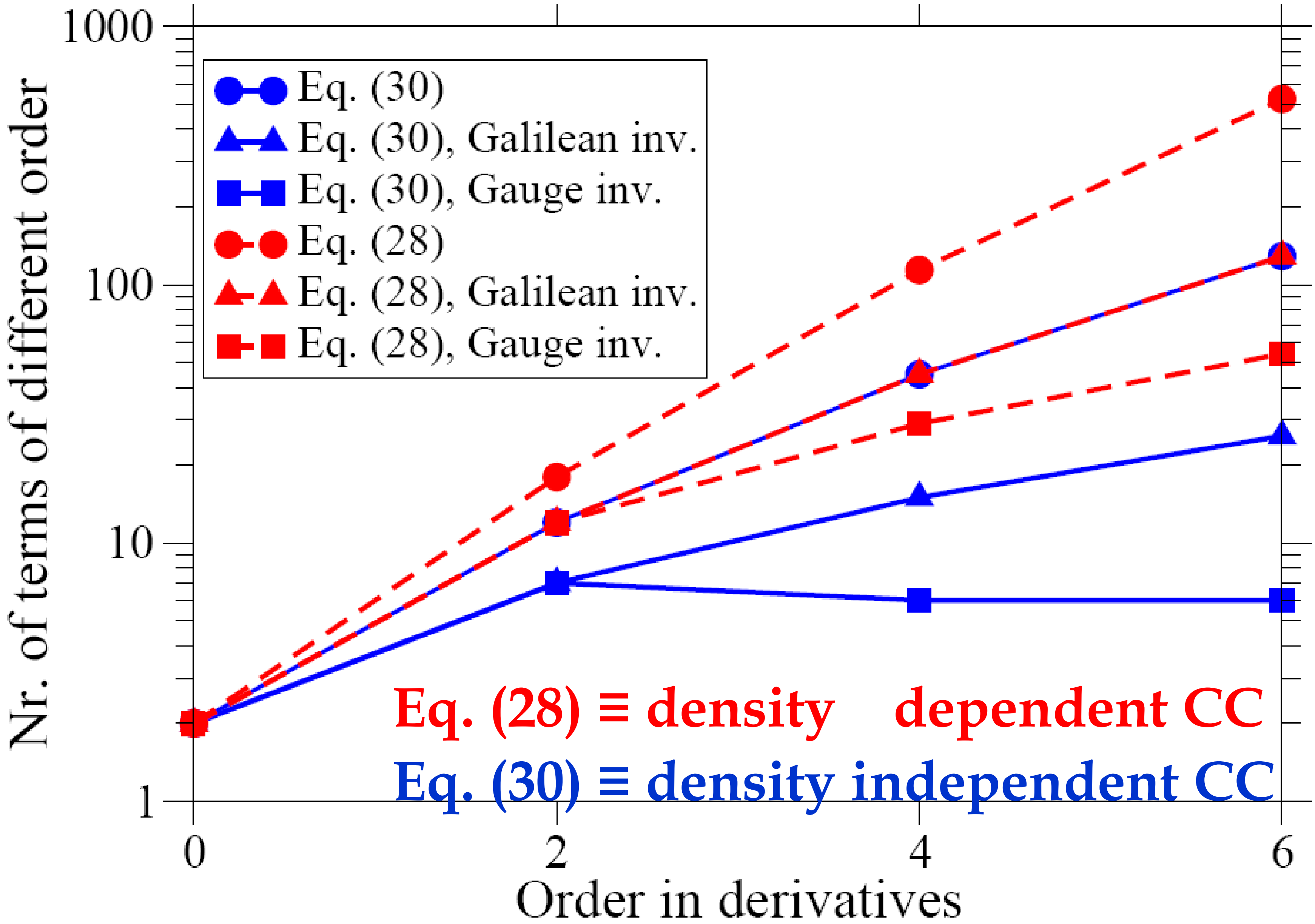
$$\nabla = \nabla_1 + \nabla_2, \qquad k = \frac{1}{2i}\left(\nabla_1 - \nabla_2\right),$$

$$\rho_{v=0} = \rho(r_1, r_2), \qquad \rho_{v=1} = \vec{s}(r_1, r_2),$$

$$\rho_{nLvJ} = \left((\vec{k}^n)_L\rho_v\right)_J \text{ (primary)}, \ \rho_{mInLvJQ} = \left((\vec{\nabla}^m)_I\left((\vec{k}^n)_L\rho_v\right)_J\right)_Q \text{ (secondary)}$$

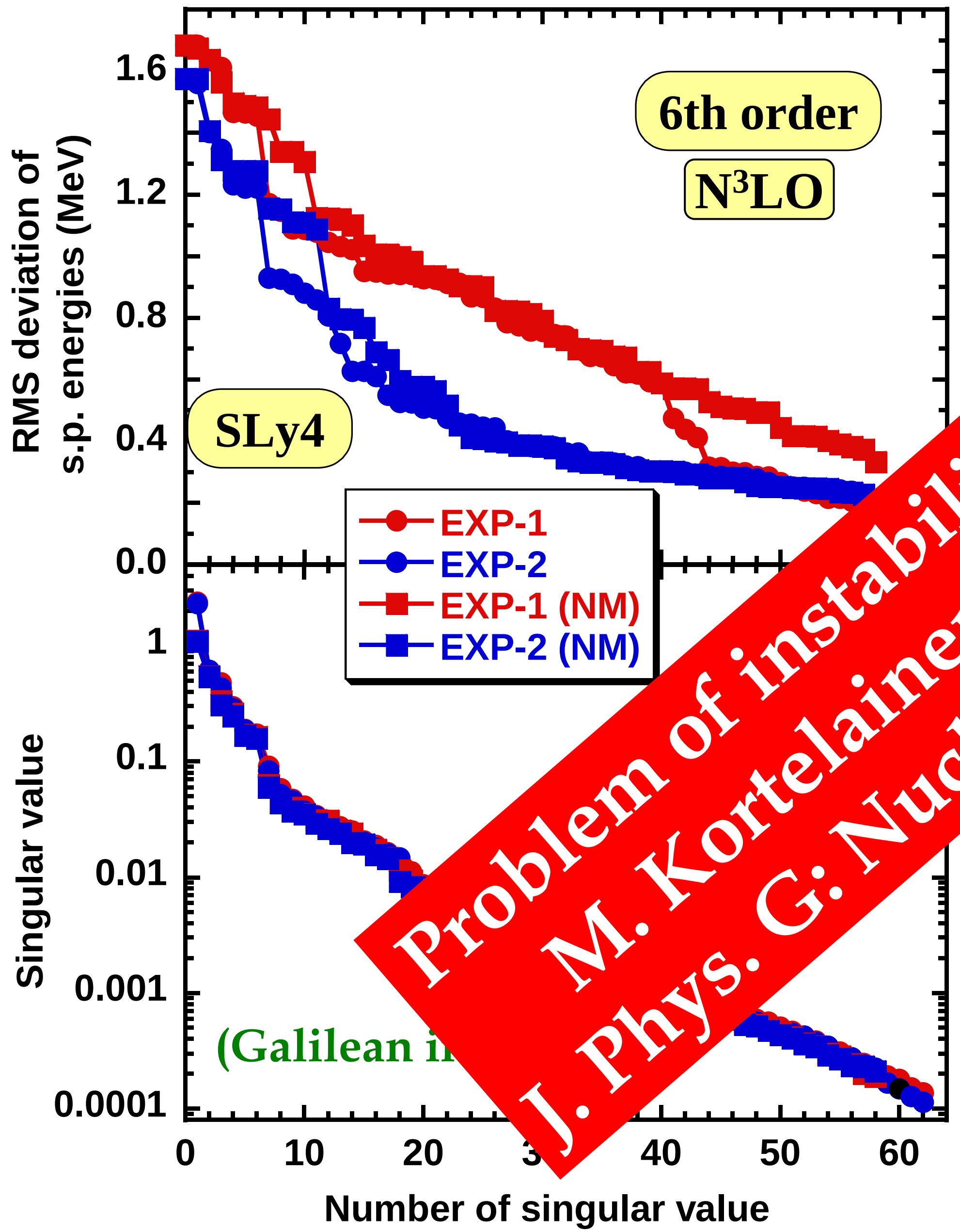
B.G. Carlsson *et al.*, Phys. Rev. C 78, 044326 (2008)

Numbers of terms in the density functional up to N^{3}LO



B.G. Carlsson *et al.*, Phys. Rev. C 78, 044326 (2008)

Fits of s.p. energies – regression analysis



B.G. Carls… published

EXP-1:
M.N…
I. … and
…0709.3525

…orquet *et al.*,
…be published

NM:
Nuclear-matter constraints on:
- saturation density
- energy per particle
- incompressibility
- effective mass

Problem of instabilities unsolved yet
M. Kortelainen and T. Lesinski
J. Phys. G: Nucl. Part. Phys. 37 064039

Challenges

Collectivity

beyond mean field, ground-state correlations, shape coexistence, symmetry restoration, projection on good quantum numbers, configuration interaction, generator coordinate method, multi-reference DFT, etc….

$$E = \langle\Psi|\hat{H}|\Psi\rangle \simeq \int\!\!\int \mathrm{d}\vec{r}\,\mathrm{d}\vec{r}\,'\,\mathcal{H}(\rho(\vec{r},\vec{r}\,'))$$

$$\text{for} \quad \rho(\vec{r},\vec{r}\,') = \frac{\langle\Psi|a^{+}(\vec{r}\,')a(\vec{r}\,')|\Psi\rangle}{\langle\Psi|\Psi\rangle}$$

True for mean field $\Downarrow$

$$\langle\Psi_1|\hat{H}|\Psi_2\rangle \simeq \int\!\!\int \mathrm{d}\vec{r}\,\mathrm{d}\vec{r}\,'\,\mathcal{H}(\rho_{12}(\vec{r},\vec{r}\,'))$$

$$\text{for} \quad \rho_{12}(\vec{r},\vec{r}\,') = \frac{\langle\Psi_1|a^{+}(\vec{r}\,')a(\vec{r}\,')|\Psi_2\rangle}{\langle\Psi_1|\Psi_2\rangle}$$

Extensions

★ **I. Range separation and exact long-range effects**

$$\mathcal{H}(\rho) = \mathcal{H}_{\text{long}}(\rho) + \mathcal{H}_{\text{short}}(\rho)$$

★ **II. Derivatives of higher order:**

$$\mathcal{H}(\rho) = \mathcal{H}(\rho, \tau, \tau_4, \tau_6, \Delta\rho, \Delta^2\rho, \Delta^3\rho, \ldots)$$

★ **III. Products of more than two densities:**

$$\mathcal{H}(\rho) = \mathcal{H}(\rho^2, \rho^3, \tau^2, \tau^3, \rho\tau, \rho^2\tau, \ldots)$$

Synopsis and take-away messages

Nuclear EDF methods:

- provide us with universal understanding of global low-energy nuclear properties and feature an impressive array of applications.
- may be rooted in the effective-theory approach whereupon low-energy phenomena can be successfully modeled without resolving high-energy properties.
- strongly rely upon and use the continuous progress in high-power computing.
- must be transformed from modeling to theory by working out consistent scheme of consecutive corrections that would allow for the increased precision and predictive power.