EMMI Rapid Reaction Task Force: “Nuclear physics confronts relativistic collisions of isobars”

Relativistic energy density functionals

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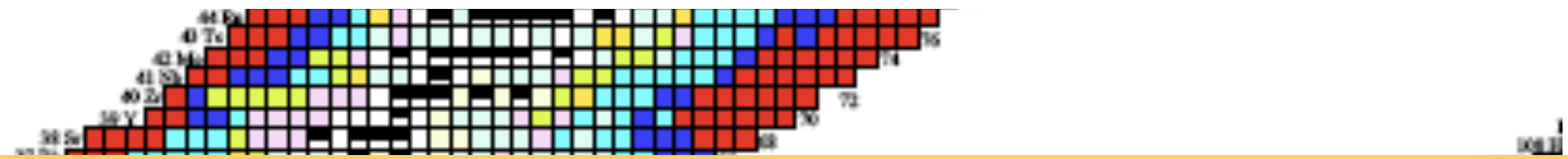
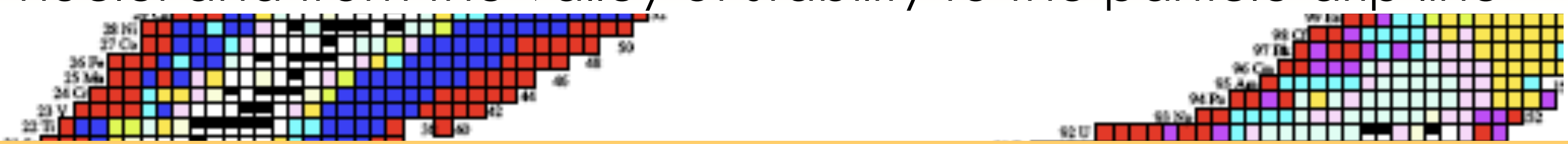
Theory framework: Energy Density Functionals

✔ the nuclear many-body problem is effectively mapped onto a one-body problem without explicitly involving internucleon interactions

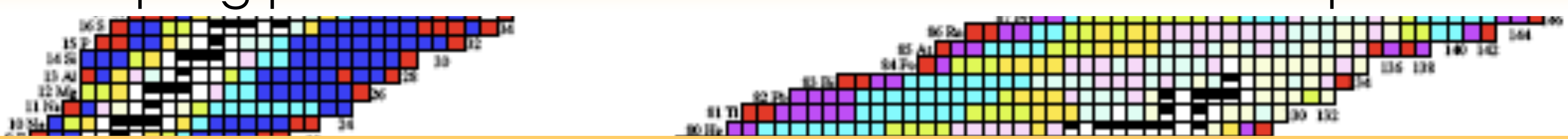
✔ the exact density functional is approximated with powers and gradients of ground state densities and currents



✔ universal density functionals can be extended from relatively light systems to superheavy nuclei and from the valley of stability to the particle drip line



✔ the coupling parameters of the EDF are fine-tuned to empirical data



✔ covariant EDFs – built from densities and currents bilinear in the Dirac spinor field of the nucleon

Theory framework: Energy Density Functionals

Meson-exchange models

- Nucleons are coupled by exchanging (phenomenological) mesons
- Models with density dependent meson-nucleon couplings (TW-99, DD-ME2,…)
- Models with nonlinear meson terms (NL3, NL3*, FSUGold,…)
- Initial densities → calculate meson fields → calculate potentials → solve Dirac equation → calculate densities (repeat until convergence is achieved)
- Numerically more demanding in comparison to the point-coupling models (not equally demanding for all models)

$$(-\triangle + m_\sigma^2)\sigma(\boldsymbol{r}) = -g_\sigma(\rho_v)\rho_s(\boldsymbol{r}),$$

$$(-\triangle + m_\omega^2)\omega^\mu(\boldsymbol{r}) = g_\omega(\rho_v)j^\mu(\boldsymbol{r}),$$

$$\Sigma_\phi = \mp g_\phi \phi \approx \mp \frac{g_\phi^2}{m_\phi^2}\rho_\phi \mp \frac{g_\phi^2}{m_\phi^4}\triangle\rho_\phi + \cdots .$$

PHYSICAL REVIEW C **77**, 034302 (2008)

Finite- to zero-range relativistic mean-field interactions

Point-coupling models

- Built from the four-fermion (contact) interaction terms in the various isospin-space channels
- Couplings are either density-dependent (DD-PC1,…) or contain higher order terms (PC-PK1, PC-F1,…)
- Initial densities → calculate potentials → solve Dirac equation → calculate densities (repeat until convergence is achieved)
- Numerically less demanding in comparison to the meson-exchange models

DD-PC1 interaction

Model Lagrangian

Density dependence of the couplings

$$\alpha_i(\rho) = a_i + (b_i + c_i x)e^{-d_i x} (i \equiv S, V, TV),$$

$$\begin{aligned}\mathcal{L} = {} & \bar{\psi}(i\gamma \cdot \partial - m)\psi \\ & - \frac{1}{2}\alpha_S(\hat{\rho})(\bar{\psi}\psi)(\bar{\psi}\psi) - \frac{1}{2}\alpha_V(\hat{\rho})(\bar{\psi}\gamma^\mu\psi)(\bar{\psi}\gamma_\mu\psi) \\ & - \frac{1}{2}\alpha_{TV}(\hat{\rho})(\bar{\psi}\vec{\tau}\gamma^\mu\psi)(\bar{\psi}\vec{\tau}\gamma_\mu\psi) \\ & - \frac{1}{2}\delta_S(\partial_\nu\bar{\psi}\psi)(\partial^\nu\bar{\psi}\psi) - e\bar{\psi}\gamma \cdot A\frac{(1-\tau_3)}{2}\psi.\end{aligned}$$

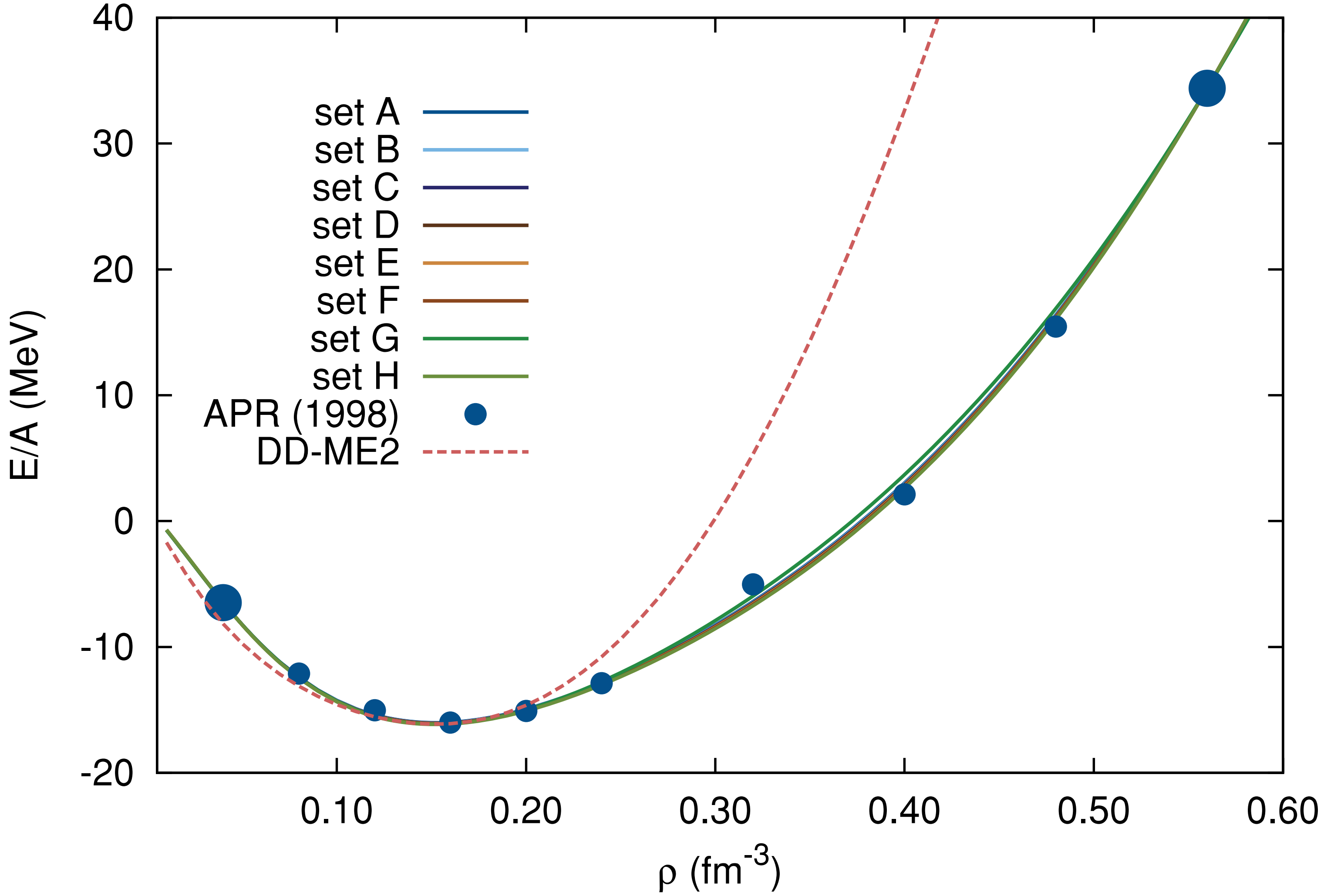
δ_s is constant

Coulomb

DD-PC1 interaction

Empirical mass formula

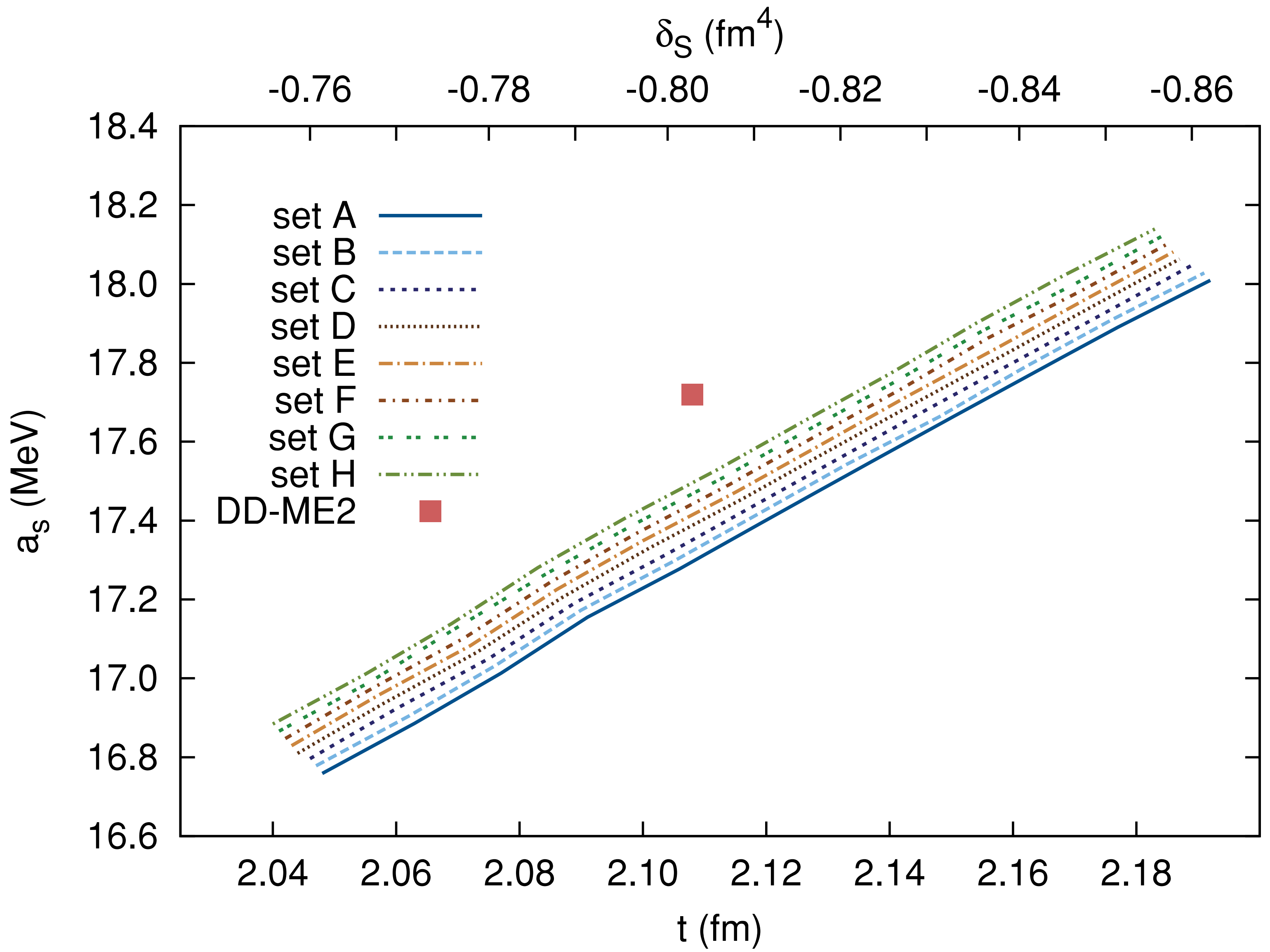
$$E_B = a_v A + a_s A^{2/3} + a_4 \frac{(N-Z)^2}{4A} + \cdots.$$



DD-PC1 interaction

Parameter of the derivative coupling

Surface energy



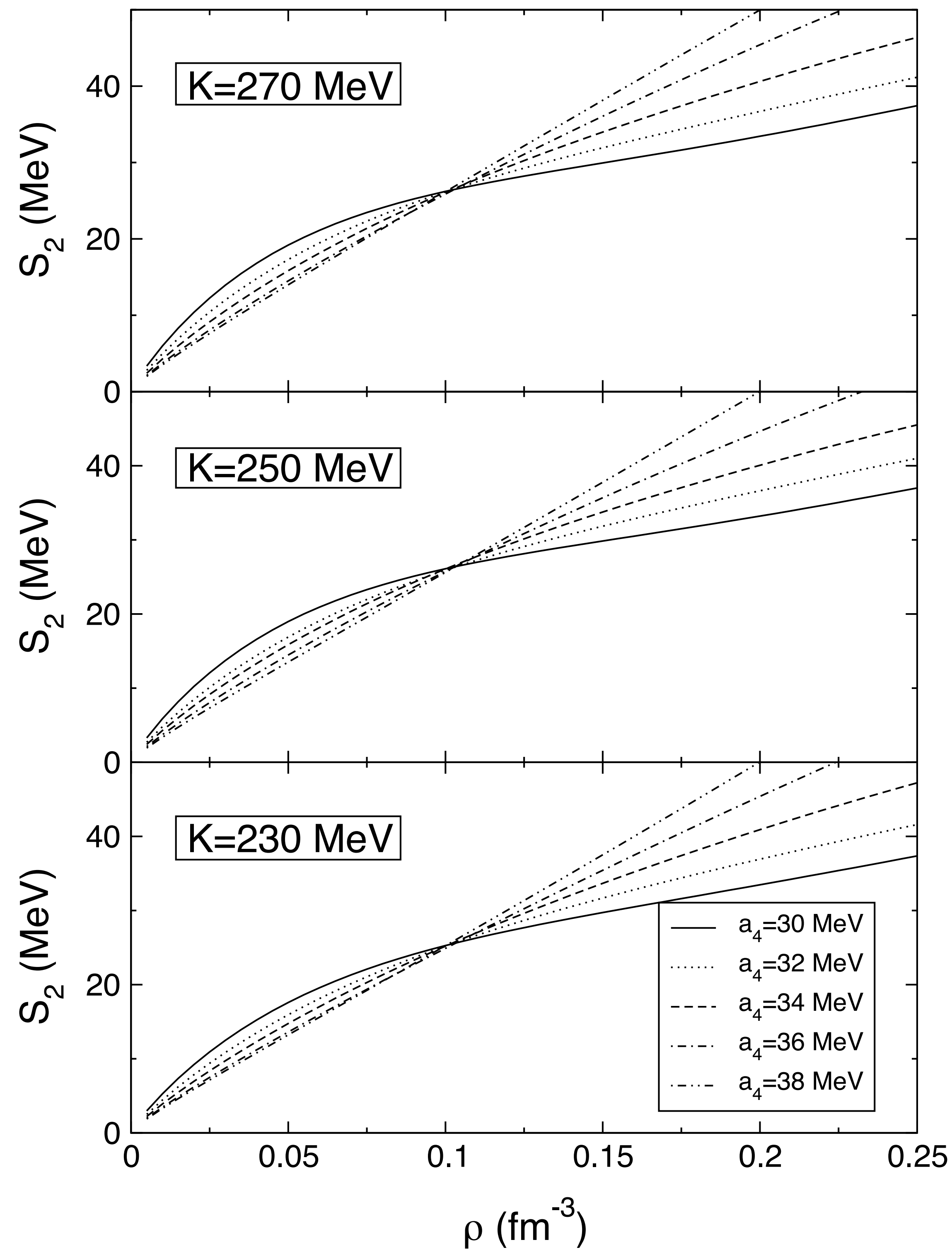
Surface thickness

DD-PC1 interaction

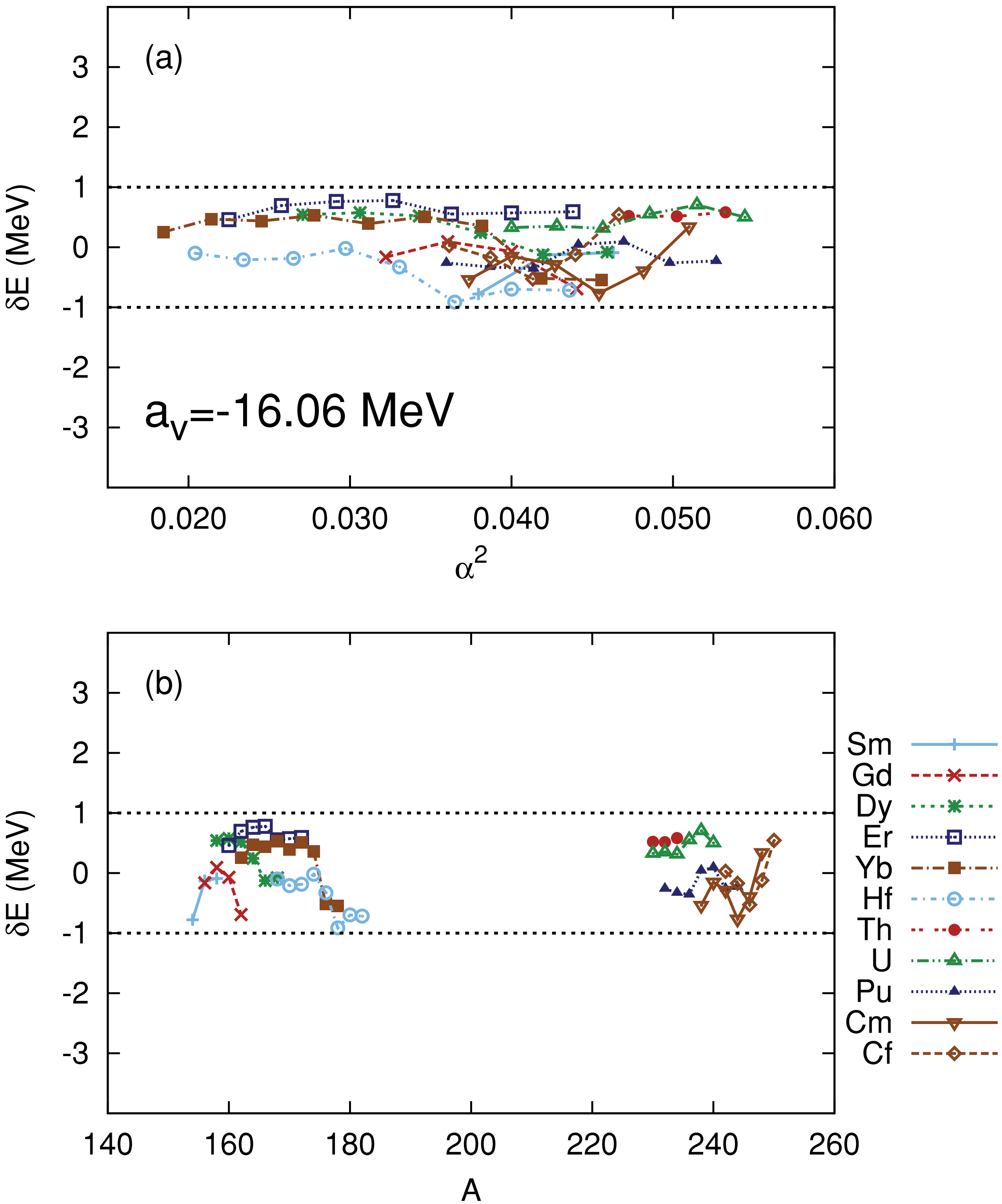
$$S_2(\rho) = a_4 + \frac{p_0}{\rho_{\rm sat}^2}(\rho - \rho_{\rm sat}) + \frac{\Delta K_0}{18\rho_{\rm sat}^2}(\rho - \rho_{\rm sat})^2 + \cdots$$

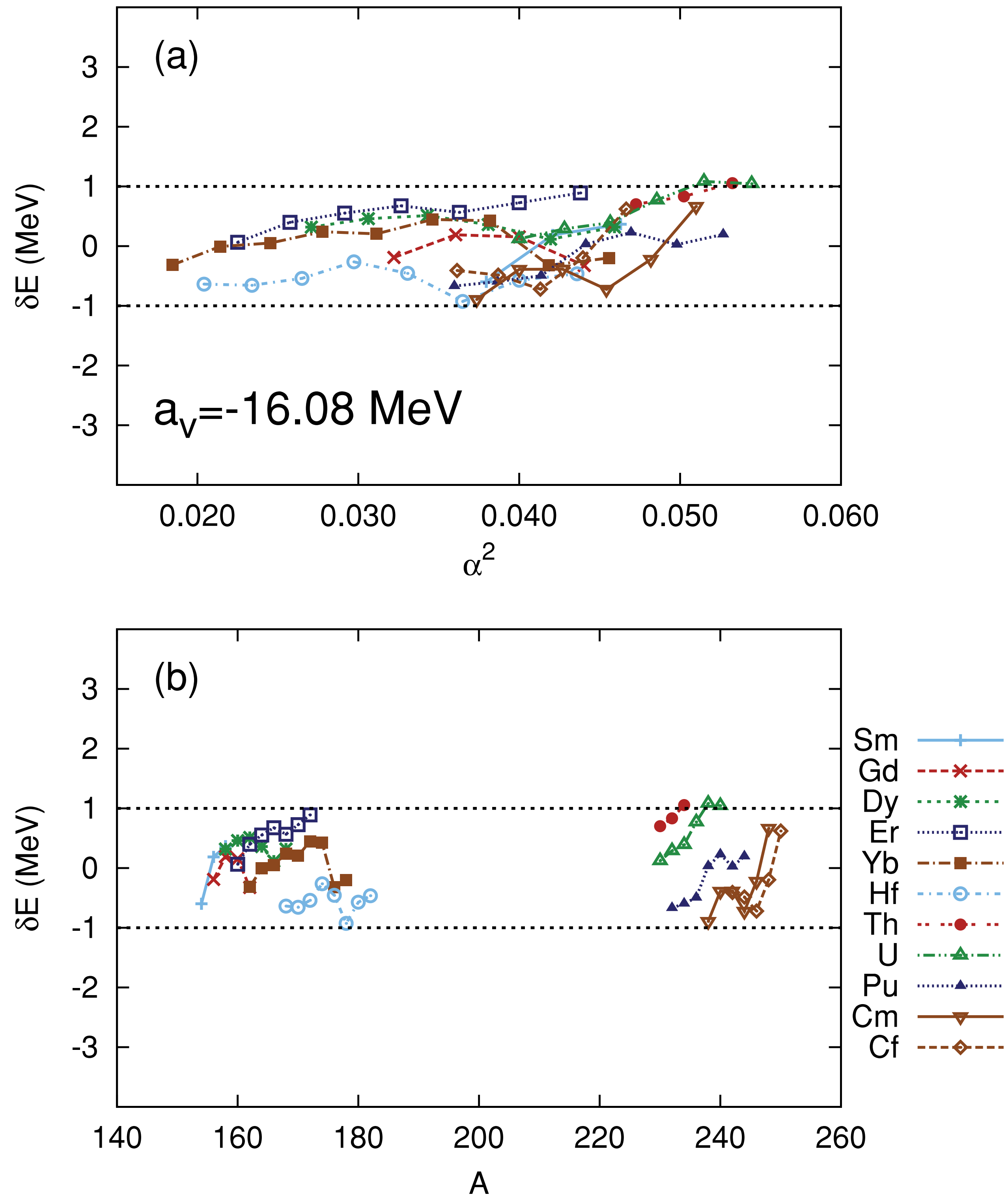
$$S_2(\rho = 0.12\ \text{fm}^{-3})$$

The binding energies constrain the value of S_2 only at the sub-saturation density $\rho=0.12$ fm^{-3}

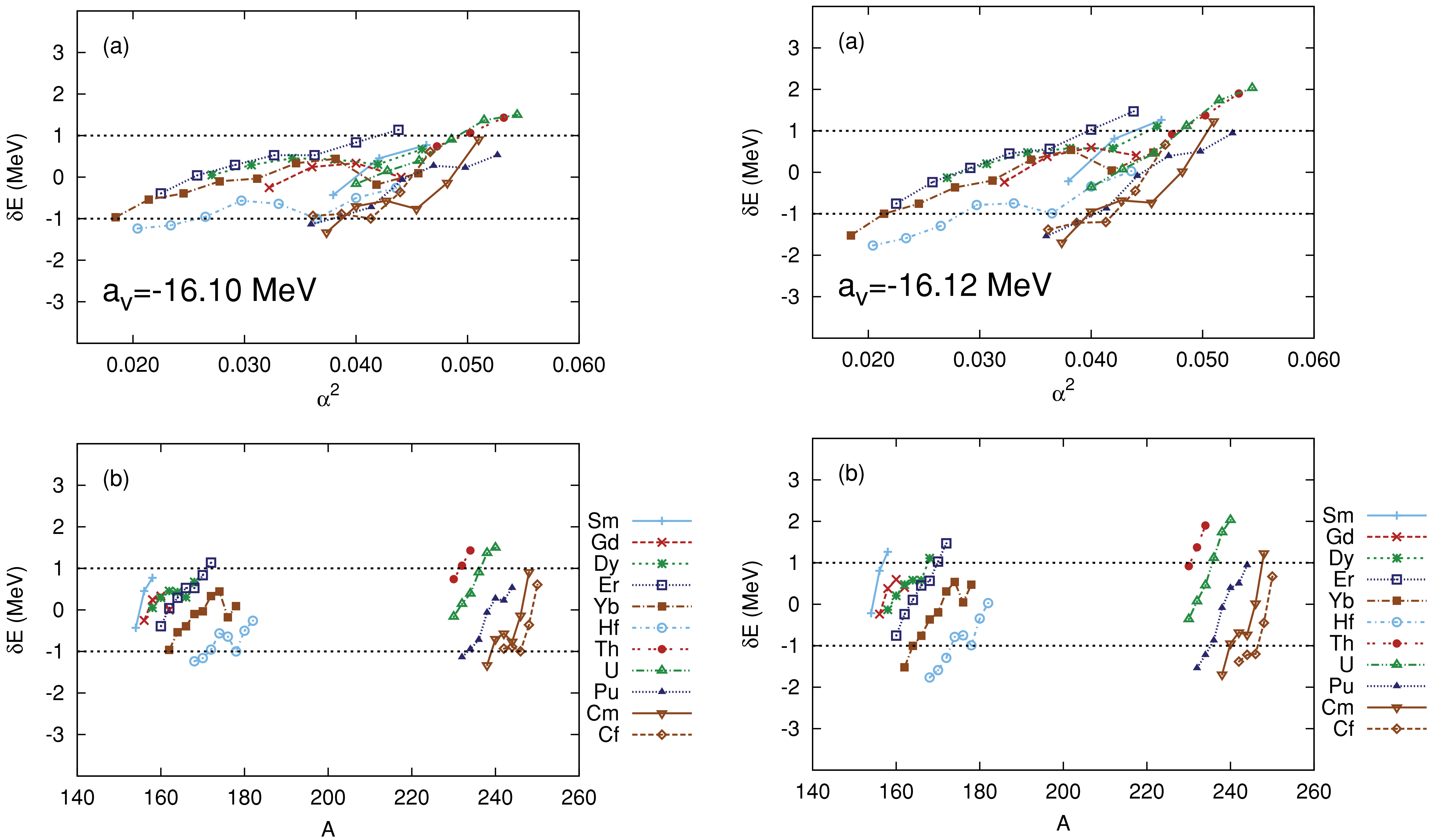


DD-PC1 interaction





DD-PC1 interaction



Some other applications…
…adjusting the EDF parameters

✓ level of accuracy (rms deviation of experimental masses) of covariant EDFs is still below the state-of-the-art non-relativistic HFB mass models:
Should additional terms be included in the EDF? (price to pay: increased model complexity)

J. Phys. G. 42, 034008 (2015)

✓ quantification of theoretical uncertainties within the EDF framework

✓ some combinations of parameters are very poorly constrained – very difficult to decouple scalar and vector channel (sum is well constrained, but not the difference)

Phys. Rev. C 95, 054304 (2017)
Phys. Rev. C 94, 024333 (2016)

✓ is it possible to systematically reduce the number of parameters defining the EDF? manifold boundary approximation method

Pairing interaction

Tian et al, Phys. Lett. B 676, 44 (2009)

- Relativistic Hartree-Bogoliubov model
- Pairing interaction: finite range separable pairing

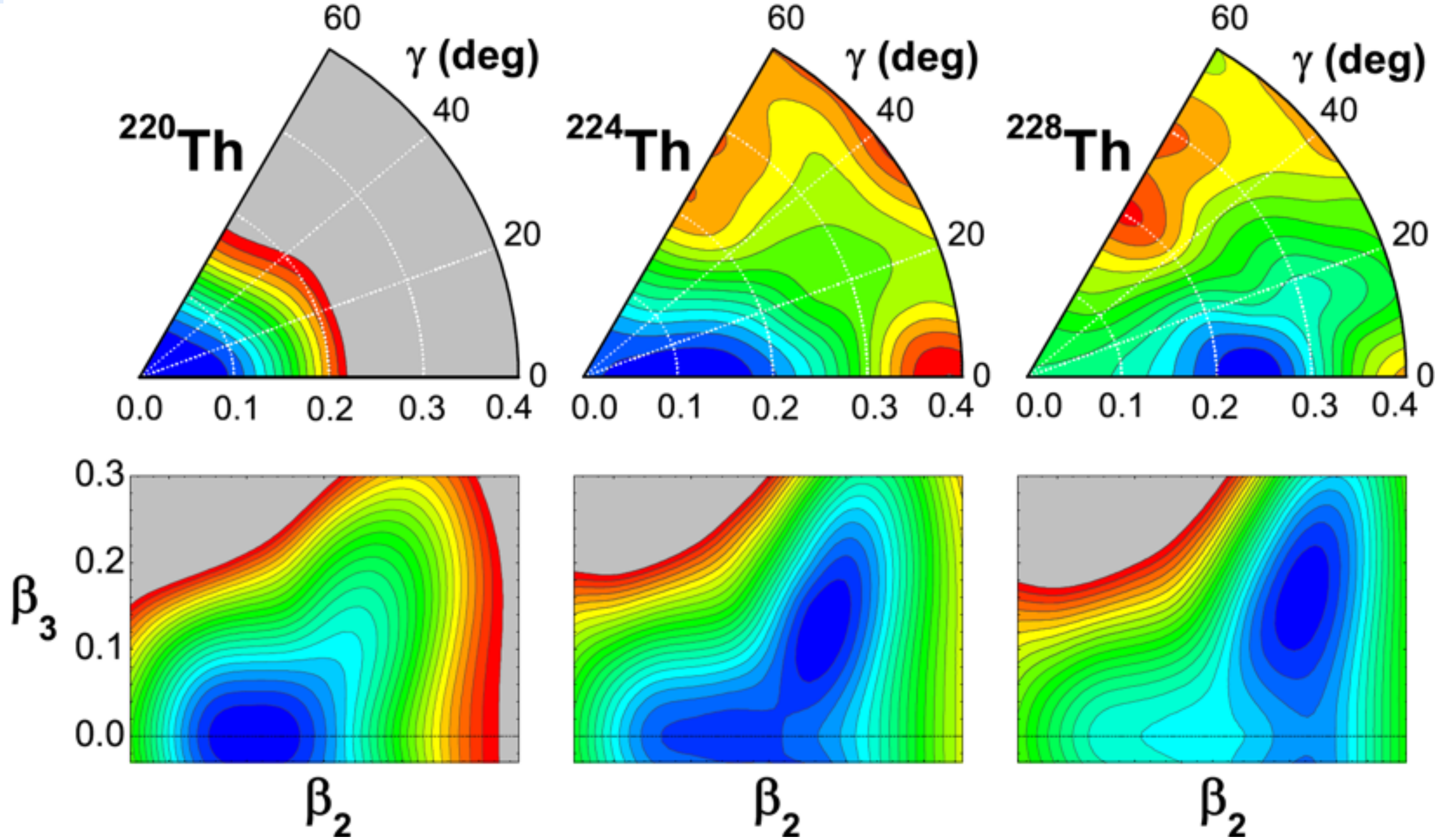
$$V(\mathbf{r}_1, \mathbf{r}_2; \mathbf{r}_1', \mathbf{r}_2') = G\delta\left(\mathbf{R} - \mathbf{R}'\right) P(\mathbf{r}) P(\mathbf{r}') \frac{1}{2}\left(1 - P^{\sigma}\right)$$

$$\mathbf{R} = \frac{1}{2}\left(\mathbf{r}_1 + \mathbf{r}_2\right), \quad \mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2, \quad P(\mathbf{r}) = \frac{1}{4\pi a^2} e^{-\frac{r^2}{4a^2}}$$

Parameters a and G are adjusted to reproduce the pairing gap in the symmetric nuclear matter calculated using the Gogny force

Basic implementation: self-consistent mean-field method

- produces energy surfaces as functions of intrinsic deformation parameters



- includes static correlations: deformations and pairing
- does not include collective correlations originating from symmetry restoration and quantum fluctuations around mean-field minima

DIRHB solver (allows for description of spherical, axial and triaxial shapes – Comp. Phys. Comm. 185, 1808 (2014) – major upgrade in preparation (parity breaking, improved computational efficiency...)

Beyond mean-field correlations: GCM

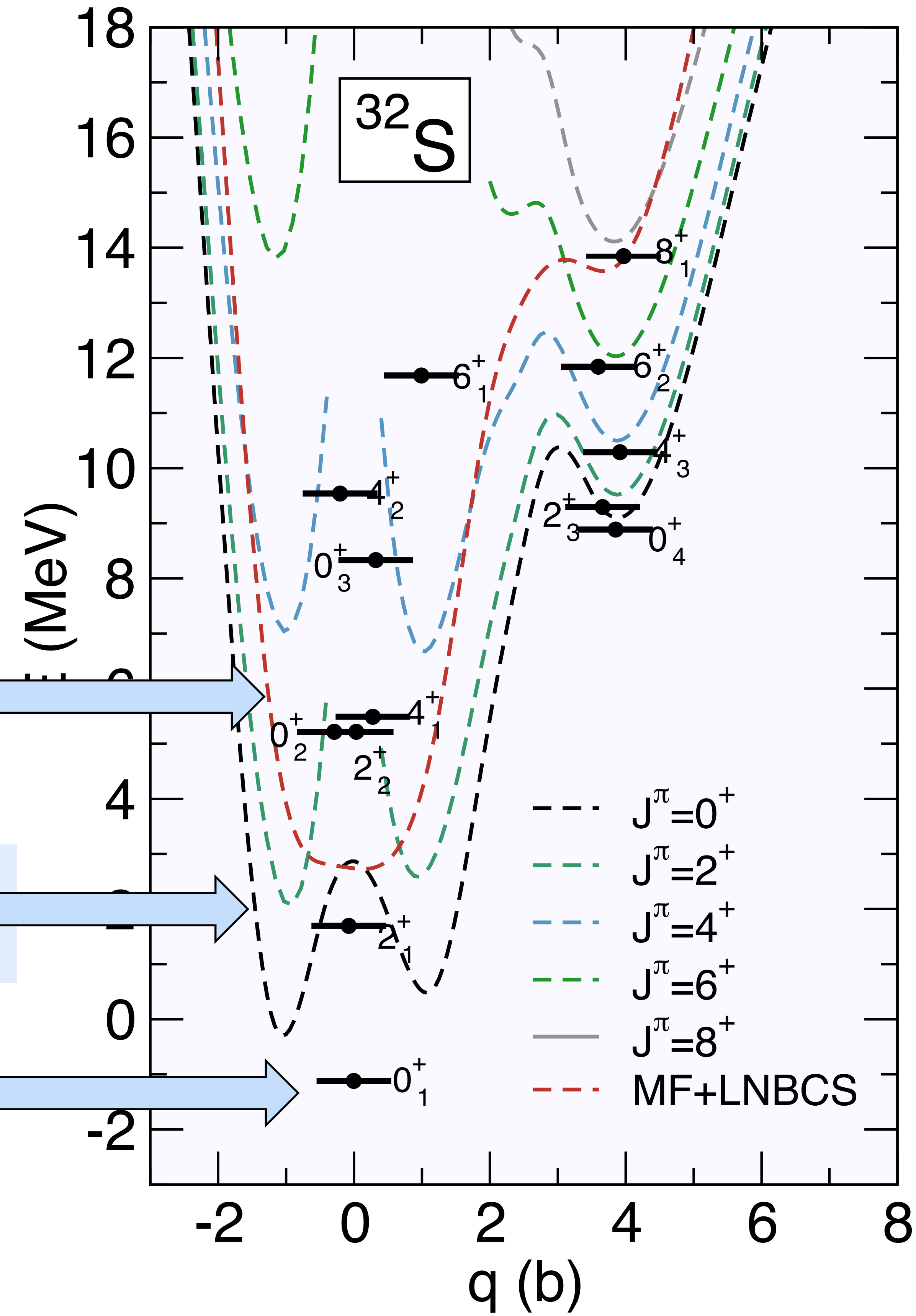
Restoration of broken symmetries (rotational, parity, particle number) and fluctuations of collective variables (quadrupole, octupole deformation)

Prog. Part. Nucl. Phys. 66, 519 (2011).
Phys. Rev. C 97, 024334 (2018).

1. Constraint mean-field calculation

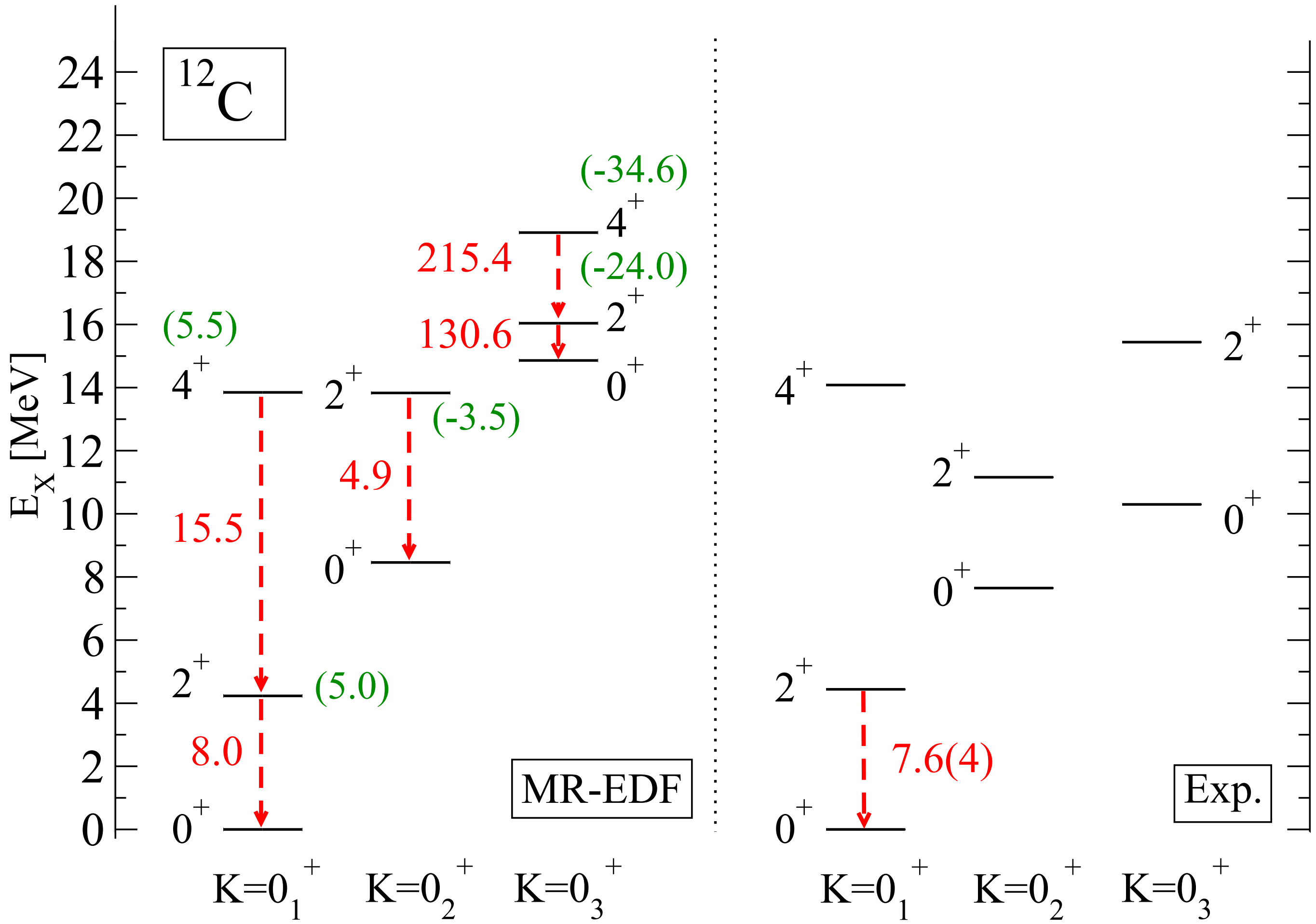
2. Angular momentum and particle number projection

3. Configuration mixing (generator coordinate method)



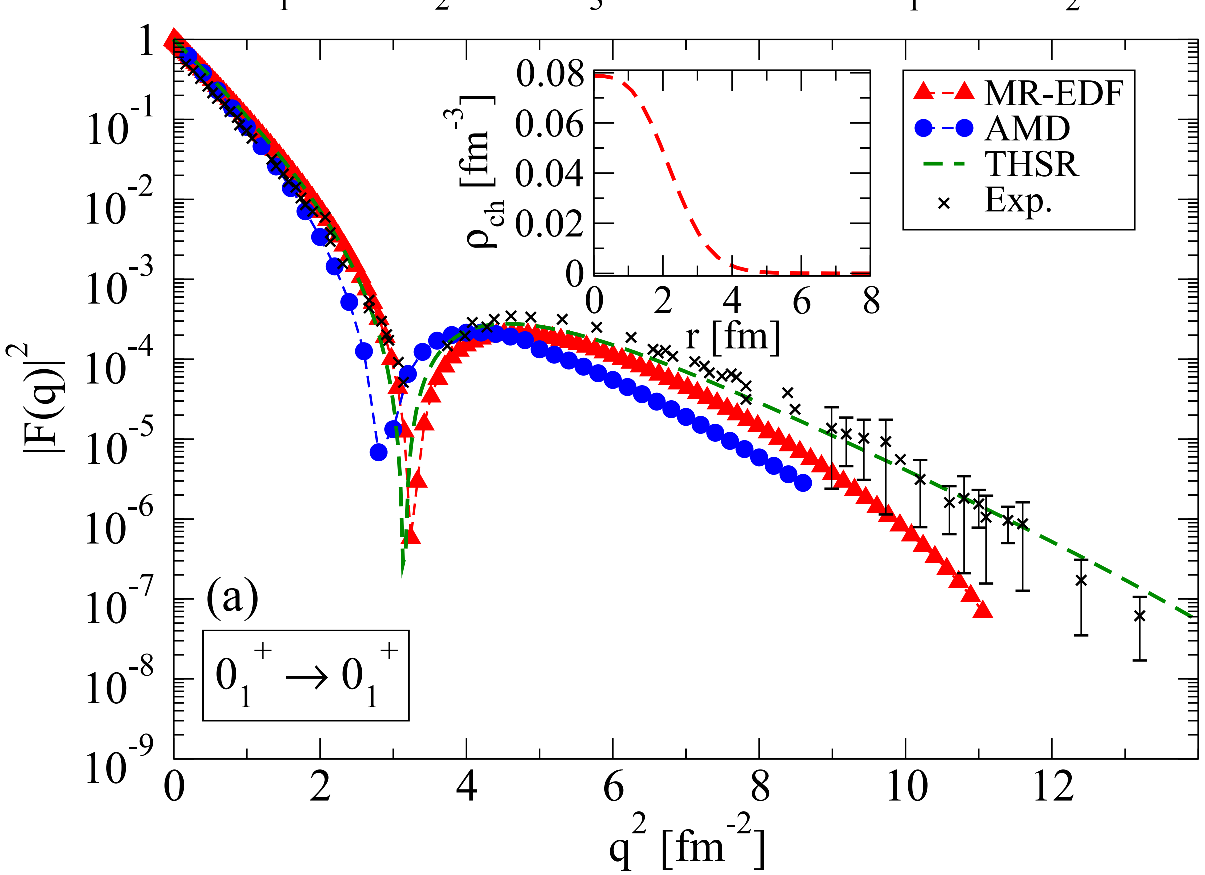
Example: description of ^{12}C isotope

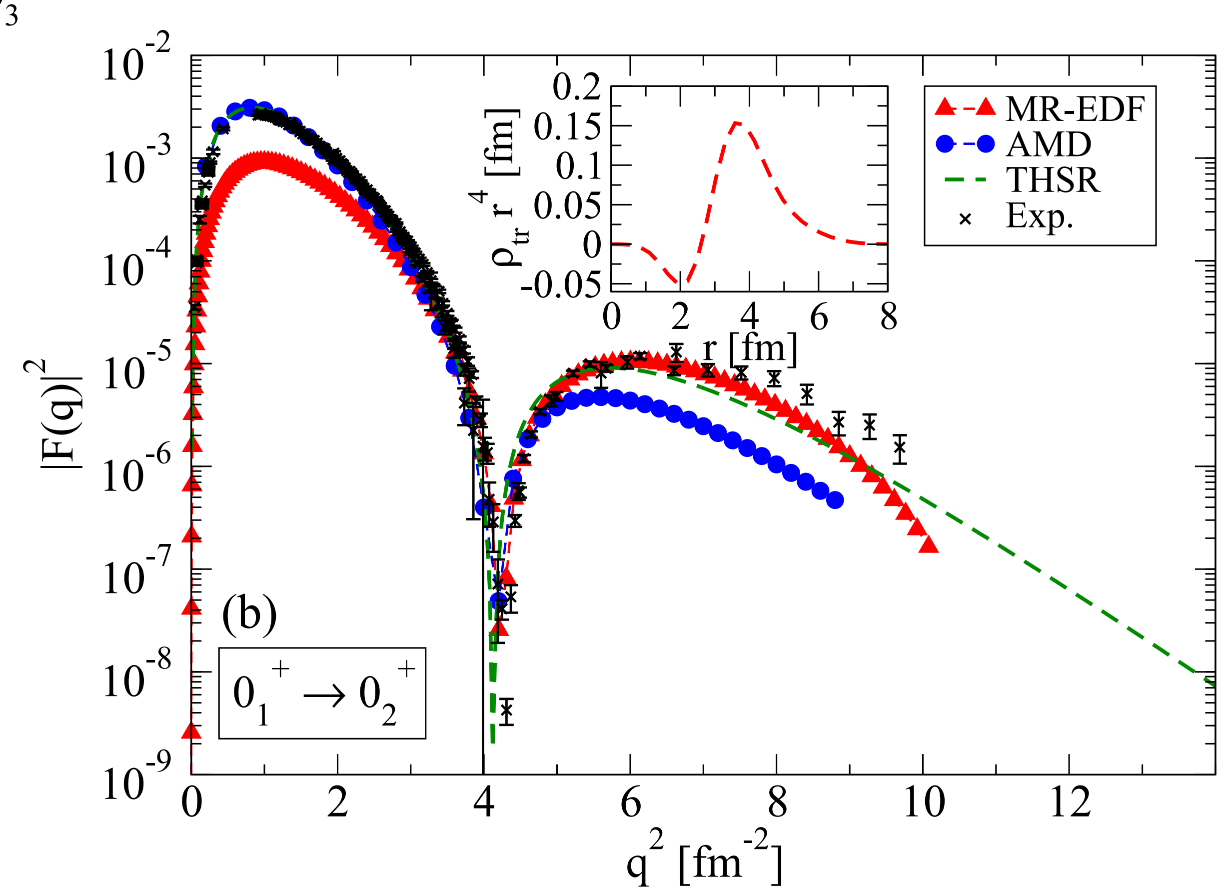
Phys. Rev. C 99, 034317 (2019)



B(E2) values in Weisskopf units

Form factors for electron scattering

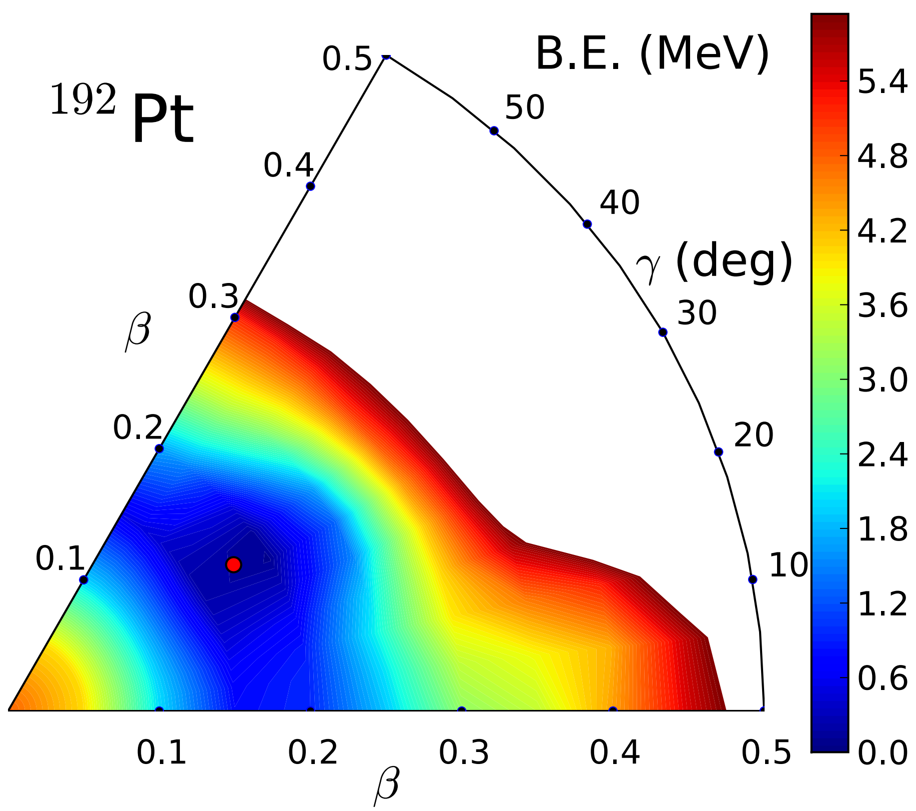




Beyond mean-field correlations: Collective Hamiltonian

Prog. Part. Nucl. Phys. 66, 519 (2011).
Phys. Rev. C 79, 034303 (2009).

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



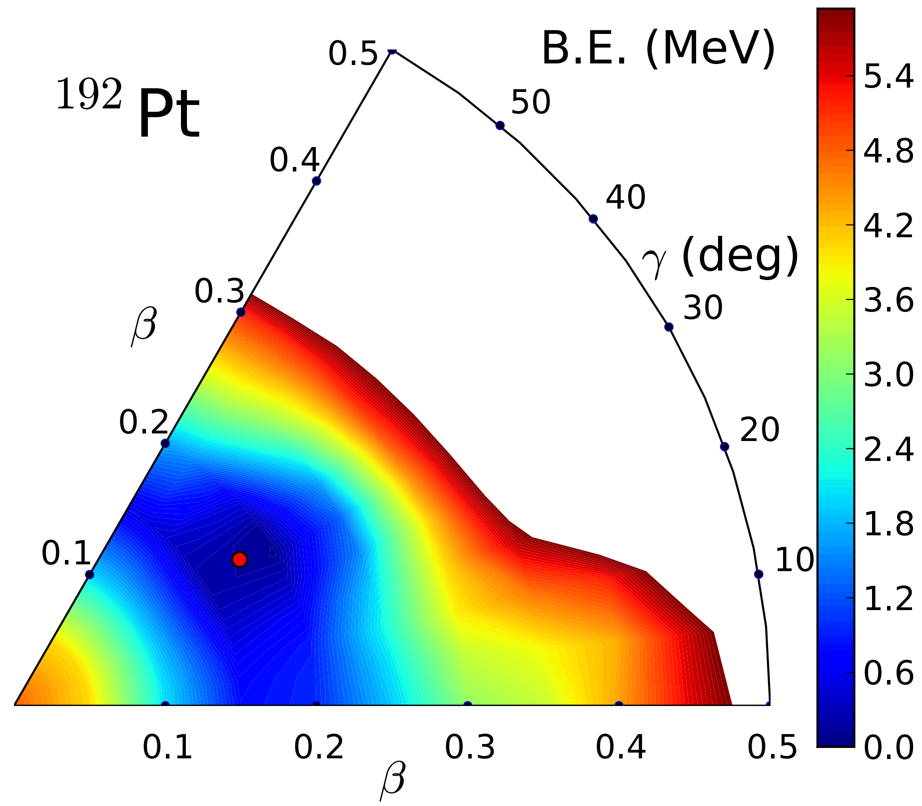
$$\mathcal{H}_{\text{coll}} = \mathcal{T}_{\text{vib}}(\beta,\gamma) + \mathcal{T}_{\text{rot}}(\beta,\gamma,\Omega) + \mathcal{V}_{\text{coll}}(\beta,\gamma)$$

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

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

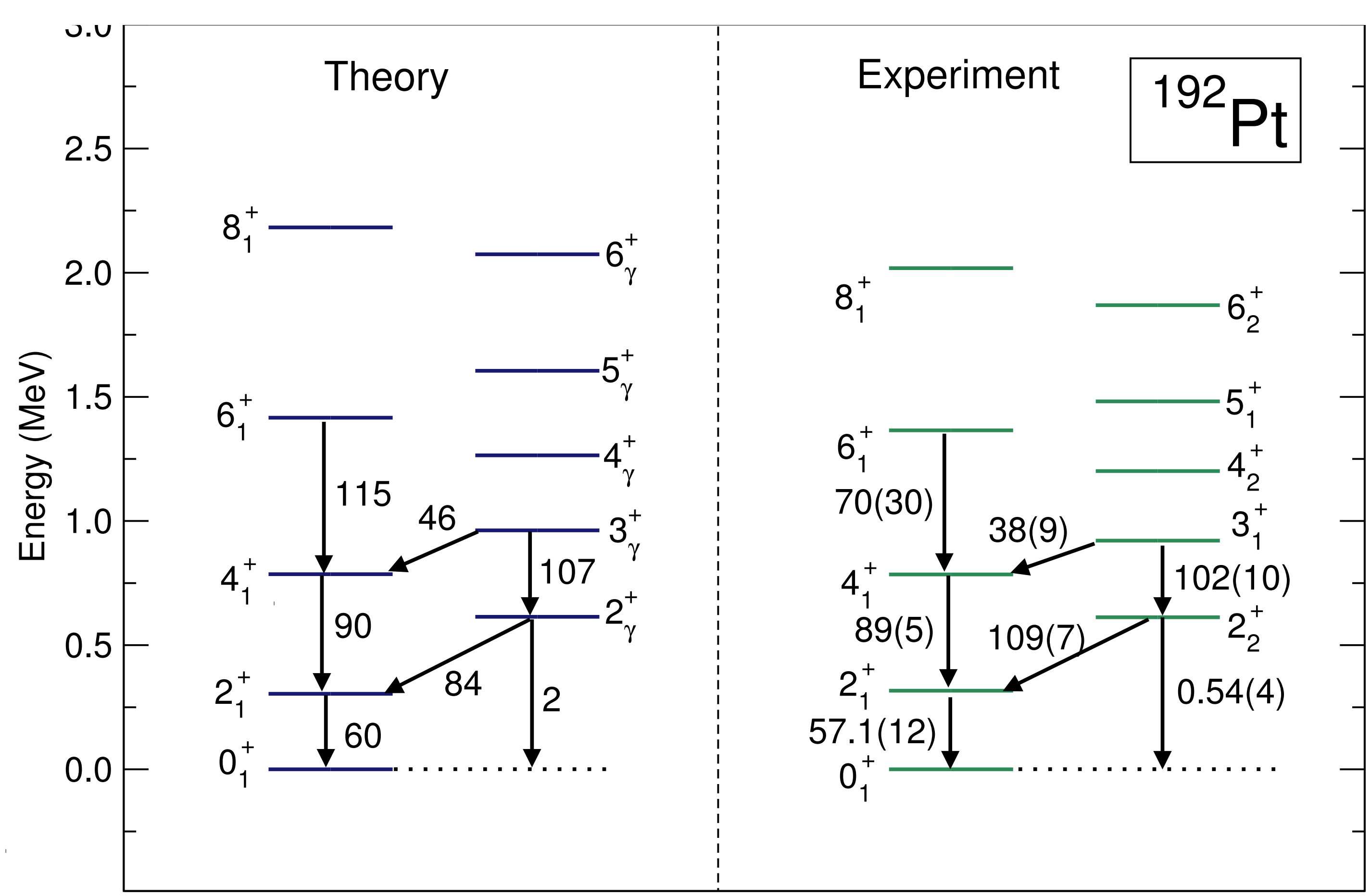
The entire dynamics of the collective Hamiltonian is governed by the seven functions of the intrinsic deformations β and γ: the collective potential, the three mass parameters: $B_{\beta\beta}$, $B_{\beta\gamma}$, $B_{\gamma\gamma}$, and the three moments of inertia I_k.

… collective eigenfunction: $\Psi_\alpha^{IM}(\beta,\gamma,\Omega) = \sum_{K\in\Delta I}\psi_{\alpha K}^{I}(\beta,\gamma)\Phi_{MK}^{I}(\Omega)$



✔ an intuitive interpretation of mean-field results in terms of *intrinsic shapes* and *single-particle states*

Prog. Part. Nucl. Phys. 66, 519 (2011).



✔ the *full model space* of occupied states can be used; no distinction between core and valence nucleons, *no need for effective charges!*

Linear response in deformed nuclei

Peru, Goutte, Phys. Rev. C 77, 044313 (2008)

D.P. Arteaga, P. Ring, Phys. Rev. C 77, 034317 (2008)

Toivanen et al, Phys. Rev. C 81, 034312 (2010)

Terasaki, Engel, Phys. Rev. C 82, 034326 (2010)

…and many more…

QRPA (Matrix implementation)

- QRPA amplitudes are calculated by diagonalizing QRPA matrix
- Dimension of the QRPA matrix increases rapidly with the size of the configuration space
- Additional cut-offs to reduce the size of the configuration space
- Not easy to change the code for different NEDFs
- Not trivial to parallelize

QRPA (Finite amplitude method)

- QRPA amplitudes X and Y are calculated iteratively
- Only restriction: number of oscillator shells
- Easy to implement various NEDFs
- Trivial parallelization – enables large scale calculations

Nakatsukasa, Yabana, Phys. Rev. C 71, 024302 (2005)

Nakatsukasa, Inakura, Yabana, Phys. Rev. C 76, 024318 (2007)

Avogadro, Nakatsukasa, Phys. Rev. C 84, 014314 (2011)

Stoitsov, Kortelainen, Nakatsukasa, Losa, Nazarewicz, Phys. Rev. C 84, 041305 (2011)

Liang, Nakatsukasa, Niu, Meng, Phys. Rev. C 87, 054310 (2013)

Kortelainen, Hinohara, Nazarewicz, Phys. Rev. C 92, 051302(2015)

Sun, Lu, Phys. Rev. C 96, 024614 (2017)

…and many more…

Linear response in deformed nuclei

$$X_{\mu\nu}(\omega) = -\frac{\delta H^{20}_{\mu\nu}(\omega) + F^{20}_{\mu\nu}(\omega)}{E_\mu + E_\nu - \omega}$$

$$Y_{\mu\nu}(\omega) = -\frac{\delta H^{02}_{\mu\nu}(\omega) + F^{02}_{\mu\nu}(\omega)}{E_\mu + E_\nu + \omega}$$

smearing width: $\omega \to \omega + i\gamma$

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particle-hole and particle-particle matrix elements

$$\begin{pmatrix} A & B \\ -B^* & -A^* \end{pmatrix} \begin{pmatrix} X \\ Y \end{pmatrix} = \omega \begin{pmatrix} X \\ Y \end{pmatrix}$$

$$R(E) = \sum_\nu B(E_\nu) \frac{\Gamma}{4\pi} \frac{\Gamma}{(E - E_\nu)^2 + (\Gamma/2)^2}$$

$$\gamma \leftrightarrow \Gamma/2$$

Linear response in deformed nuclei

QFAM amplitudes

$$X_{\mu\nu}(\omega) = -\frac{\delta H^{20}_{\mu\nu}(\omega) + F^{20}_{\mu\nu}(\omega)}{E_\mu + E_\nu - \omega}$$

$$Y_{\mu\nu}(\omega) = -\frac{\delta H^{02}_{\mu\nu}(\omega) + F^{02}_{\mu\nu}(\omega)}{E_\mu + E_\nu + \omega}$$

Induced density and pairing tensor

$$\delta\rho = UX(\omega)V^T + V^*Y(\omega)U^\dagger$$

$$\delta\kappa^{(+)}(\omega) = UX(\omega)U^T + V^*Y^T(\omega)V^\dagger$$

$$\delta\kappa^{(-)}(\omega) = V^*X^\dagger(\omega)V^\dagger + UY^*(\omega)U^T$$

Induced s.p. Hamiltonian and pairing field

$$\delta h(\omega),\ \delta\Delta^{(+)}(\omega) \text{ and } \delta\Delta^{(-)}(\omega)$$

Induced Hamiltonian

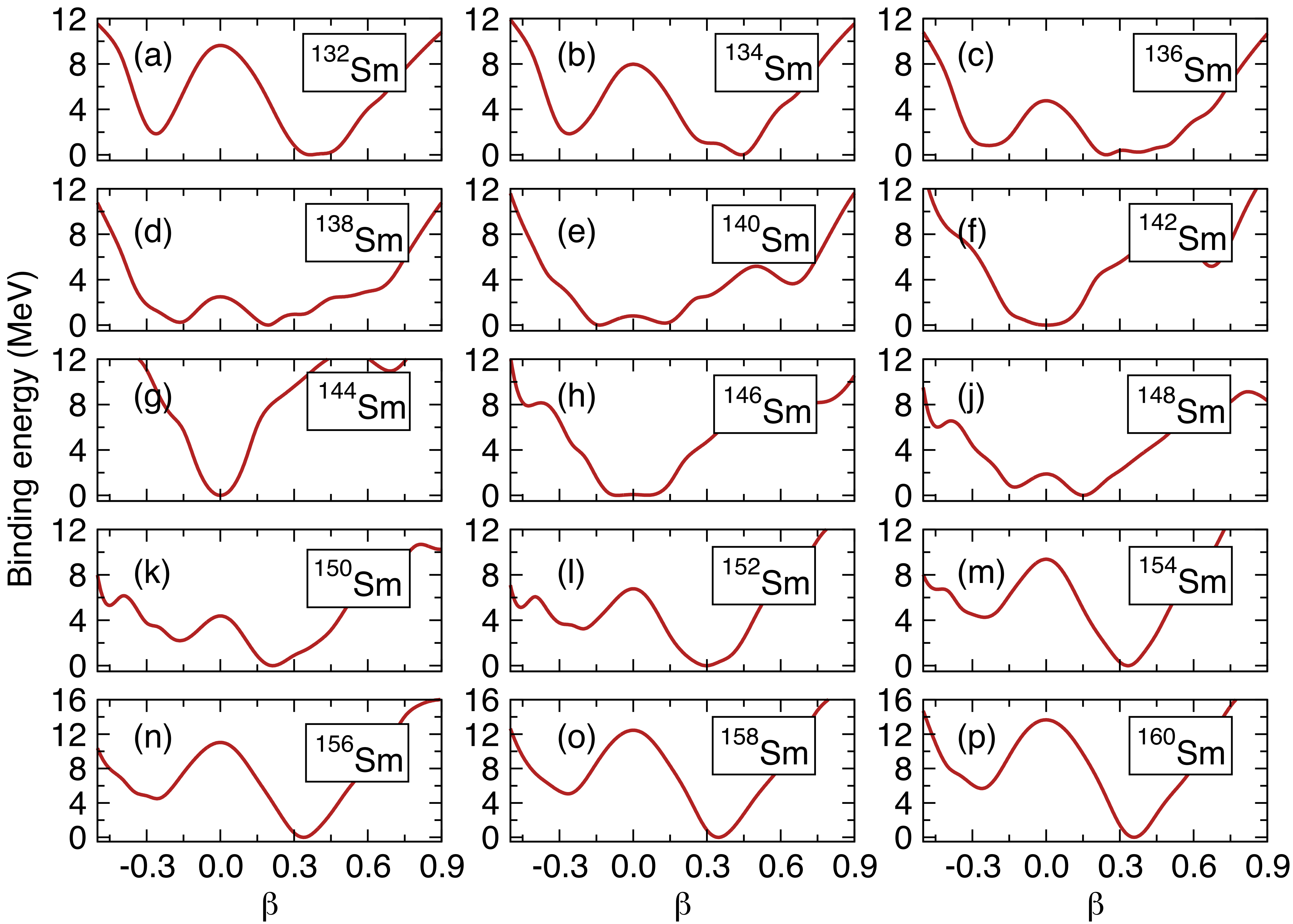
$$\delta H^{20}(\omega) \text{ and } \delta H^{02}(\omega)$$

DIRQFAM solver – Comp. Phys. Comm. 253, 107184 (2020) – major upgrade in preparation

Linear response in deformed nuclei

Sm isotopes

Phys. Rev. C 88, 044327 (2013)

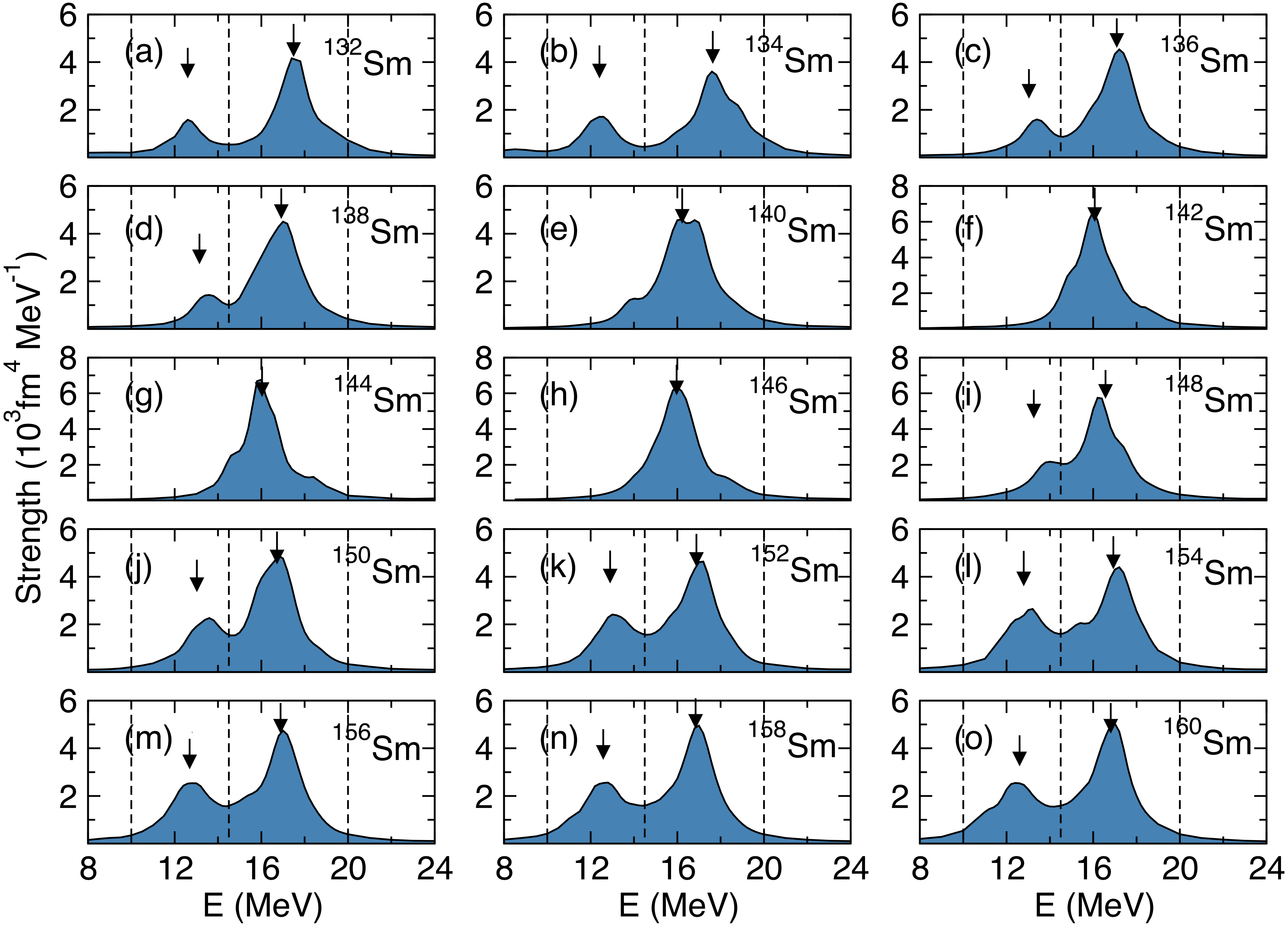


Linear response in deformed nuclei

Sm isotopes

$$K^{\pi} = 0^{+}$$ (monopole)

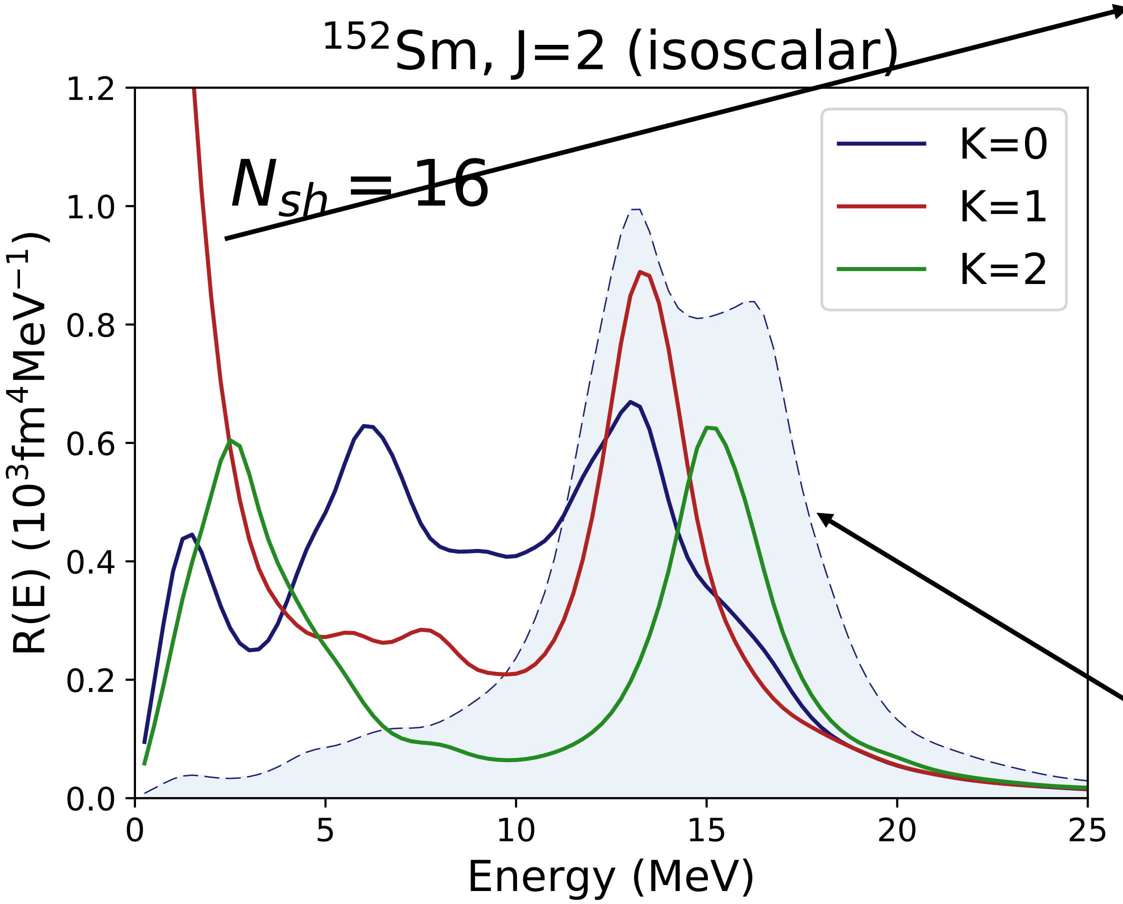
Arrows denote LE and HE centroids



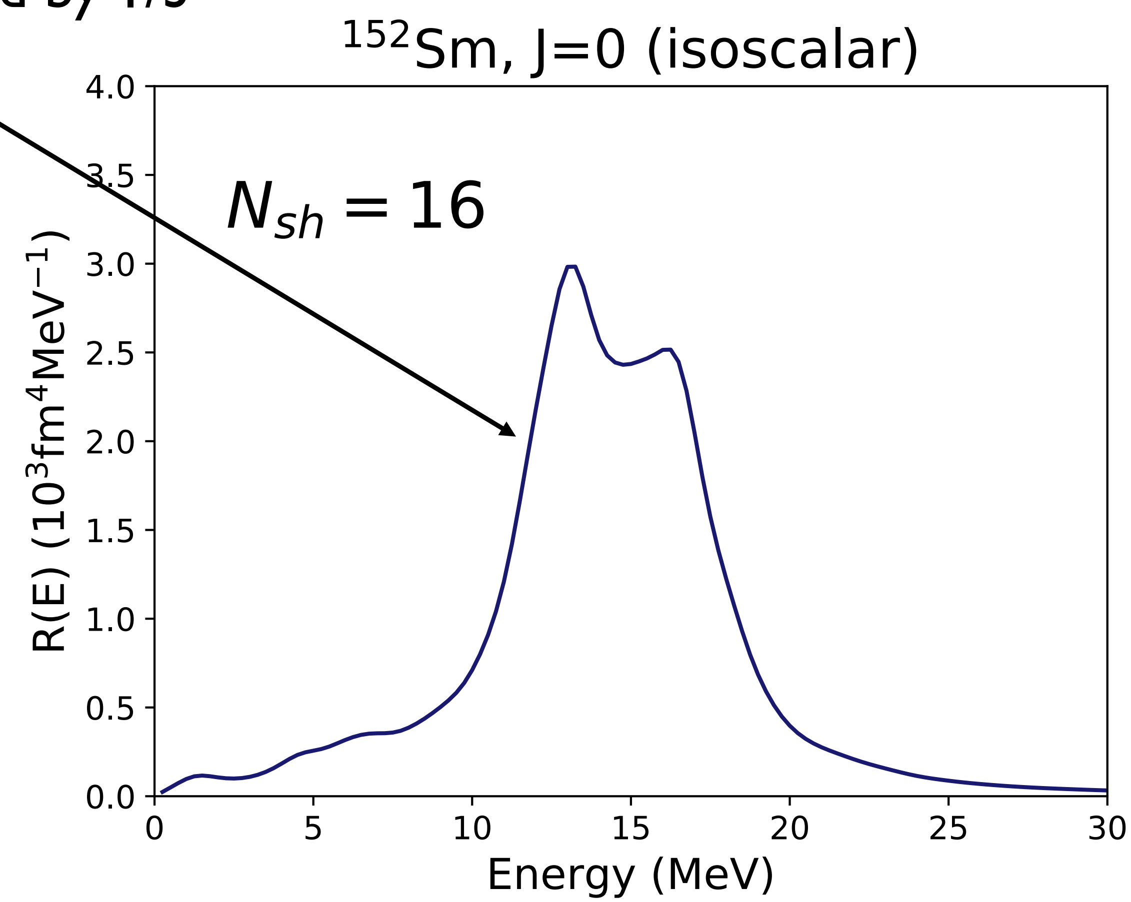
Linear response in deformed nuclei

^{152}Sm isotope

Spurious state at ~0.3 MeV



Scaled by 1/3



Itoh et al, PRC 68, 064602 (2003)

GMR

$$\mathrm{LE} : 11.27^{+0.32}_{-0.54}\ \mathrm{MeV}$$

$$\mathrm{HE} : 15.44^{+0.12}_{-0.23}\ \mathrm{MeV}$$

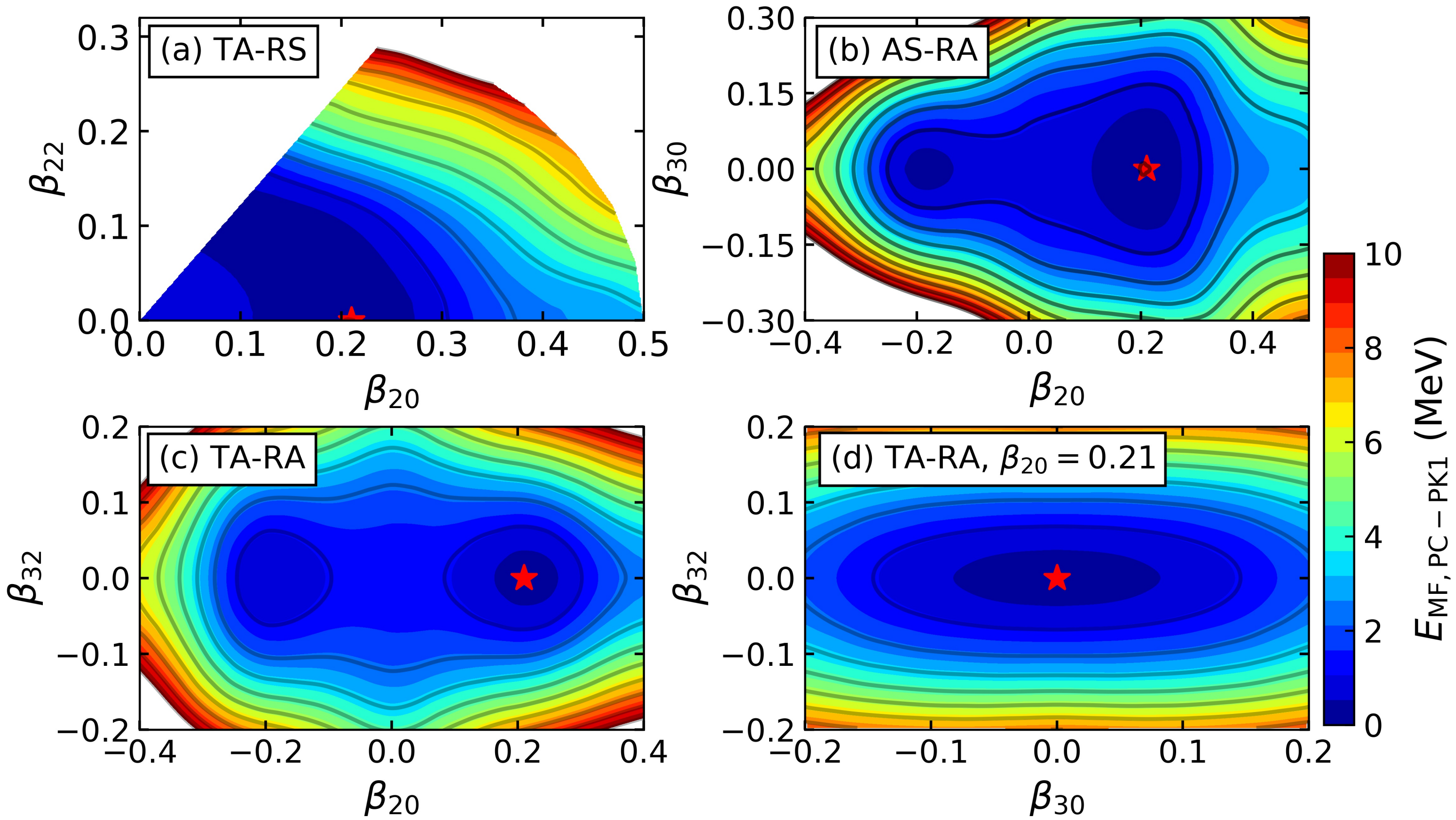
GQR

$$\mathrm{LE} : 11.53 \pm 0.14 \mathrm{MeV}$$

$$\mathrm{HE} : 14.86 \pm 0.39 \mathrm{MeV}$$

Description of ^{96}Zr within the framework of the REDFs

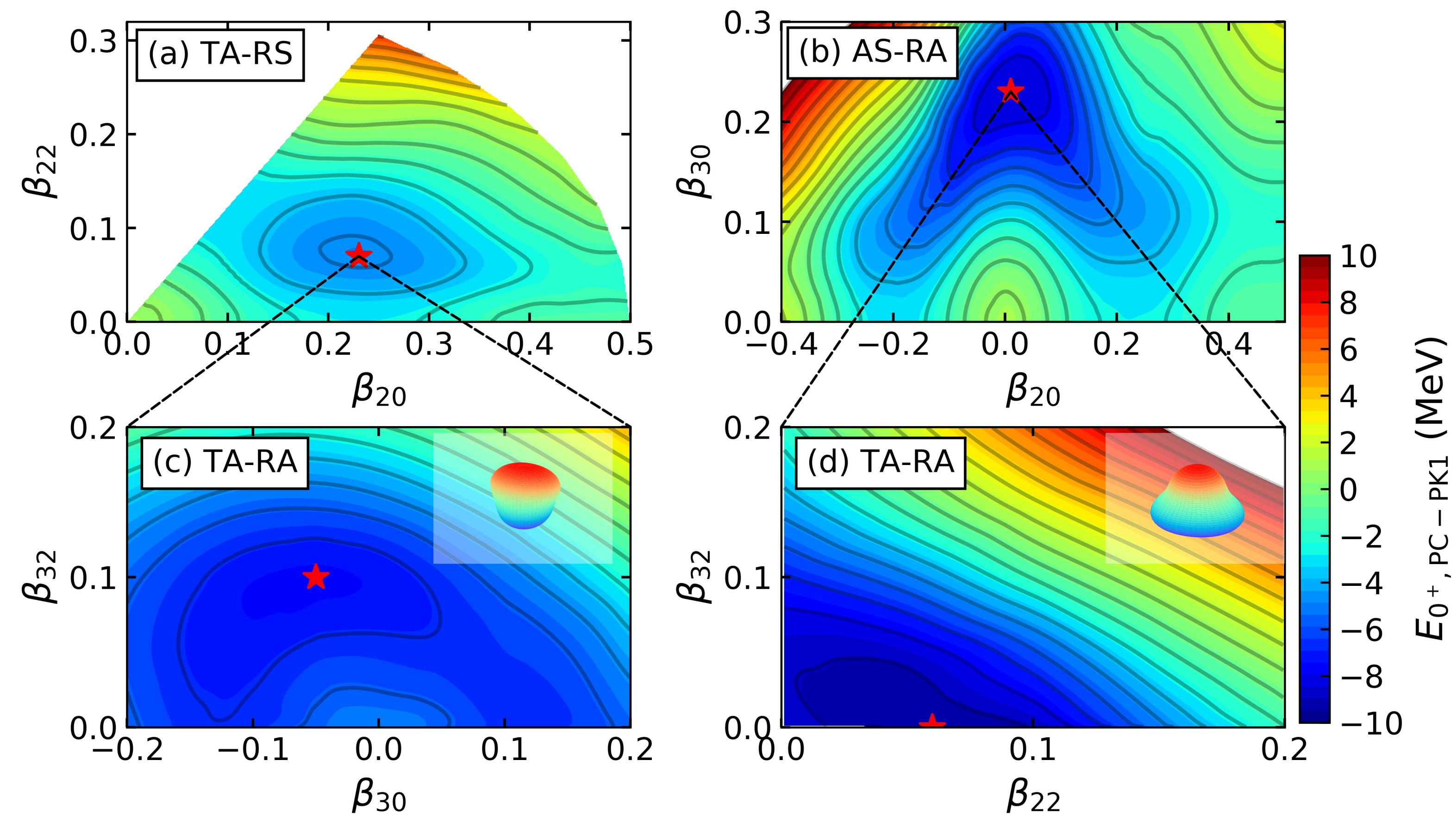
Yu-Ting Rong, Bing-Nan Lu, arXiv :2201.02114v1



Projection after variation calculation based on the multidimensionally constraint RHB model

PC-PK1 interaction (similar results are obtained with DD-PC1 or PC-F1 interactions)

Separable finite range pairing force (strength adjusted to reproduce empirical pairing gaps in ^{102,104}Zr

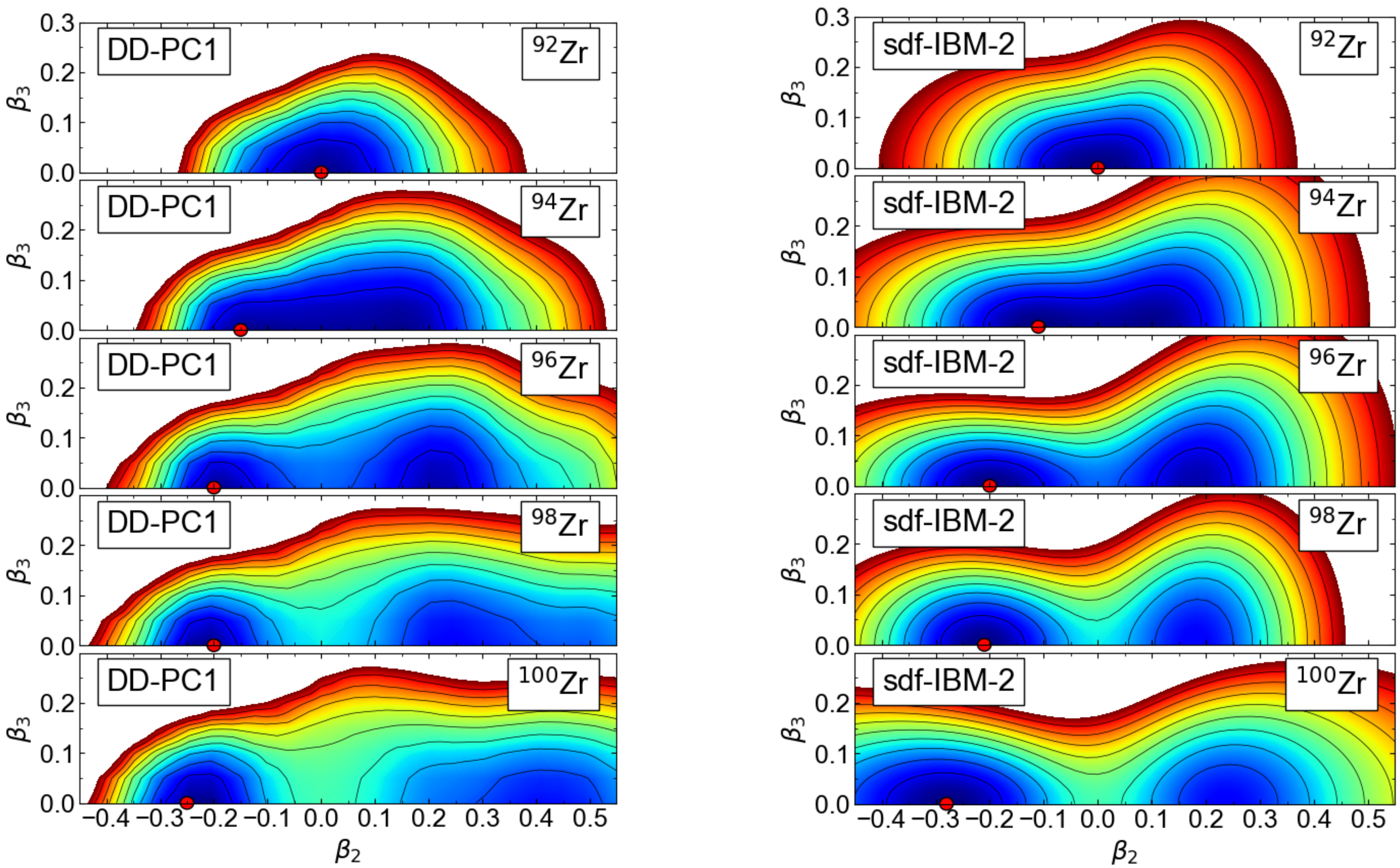


Octupole correlations in collective excitations of neutron rich N=56 nuclei

K. Nomura, Phys. Rev. C 105, 054318 (2022)

Interacting boson model based on the nuclear density functional theory

Quadrupole octupole SCMF energy surface is mapped onto the equivalent surface in the system of interacting monopole s, quadrupole d and octupole f bosons



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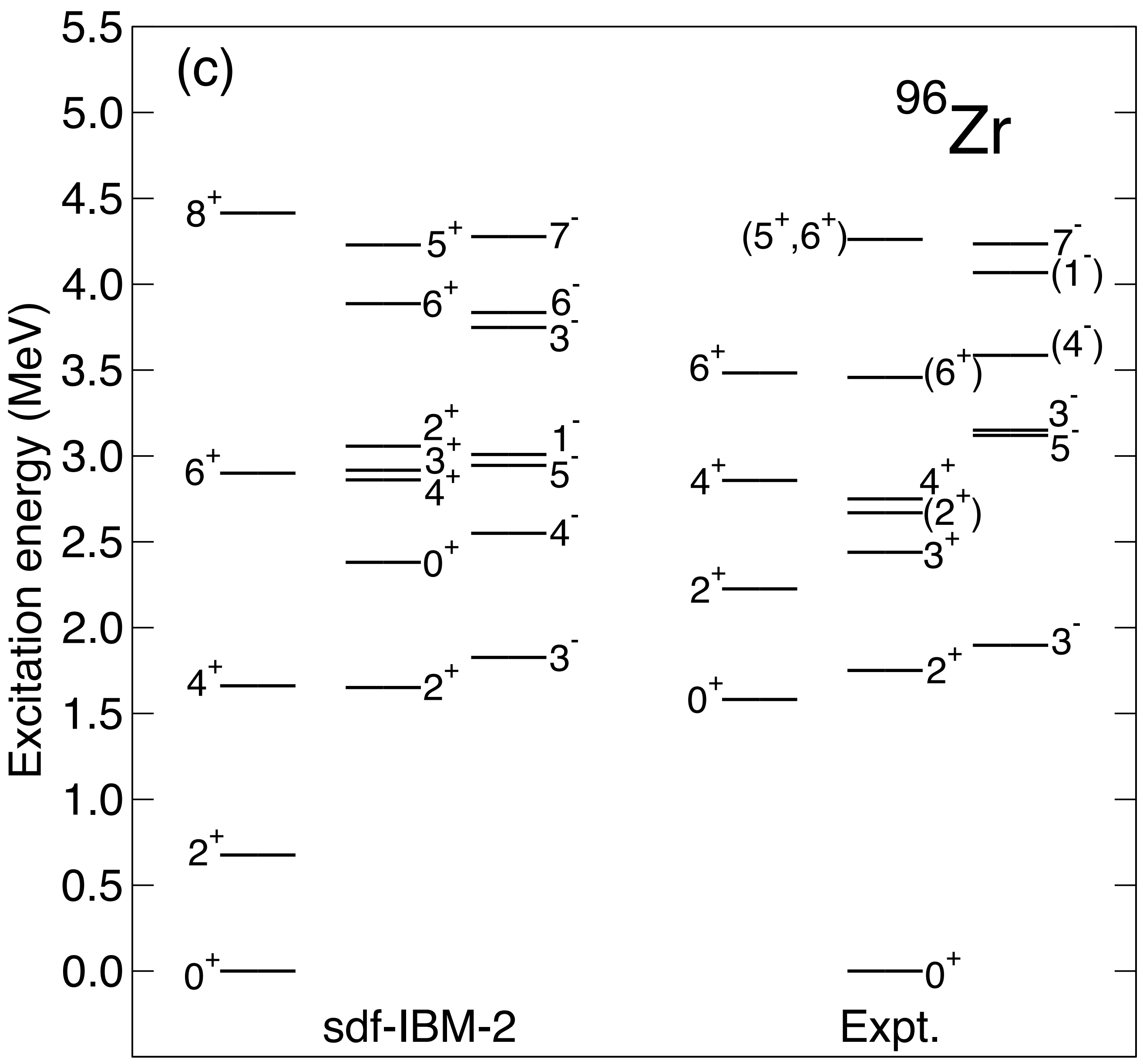

The model needs to be extended so that is simultaneously handles the octupole boson degrees of freedom, the triaxial deformation, the intruder states and configuration mixing.

Summary

✓ NEDFs provide an economic, global and accurate microscopic approach to nuclear structure that can be extended from relatively light systems to superheavy nuclei, and from the valley of β-stability to the particle drip-lines.

✓ NEDF-based structure models that take into account collective correlations → microscopic description of low-energy observables: excitation spectra, transition rates, changes in masses, isotope and isomer shifts, related to shell evolution with nuclear deformation, angular momentum, and number of nucleons.

✓ NEDF-based models are applicable to large-scale calculations