Report, code package, and tables with global ground-state observables calculated for weakly bound nuclei

Subtask 1-1: Evolution of single-particle states in function of proton and neutron numbers

Subtask 1-2: Coupling between single particle and collective modes

Subtask 1-3: Description of nuclear masses

Parameters of nuclear energy-density-functionals (EDFs) are always derived by an optimisation to experimental data. For the minima of appropriately defined penalty functions, a statistical sensitivity analysis provides the uncertainties of the EDF parameters. To quantify theoretical errors of observables given by the model, we studied the propagation of uncertainties within the UNEDF0 Skyrme-EDF approach. We found that typically the standard errors rapidly increase towards neutron rich nuclei. This can be linked to large uncertainties of the isovector coupling constants of the currently used EDFs.

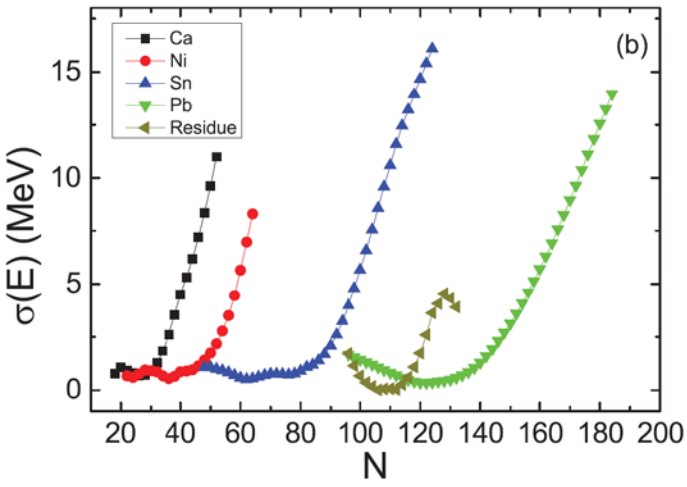

Fig. 1. Propagated errors of binding energies of semimagic nuclei, calculated for isotopic chains with magic proton numbers up to very exotic weakly bound nuclei. For the Pb nuclei, moduli of fit residuals with respect to experimental data are also shown.

Models based on using perturbative polarization corrections and mean-field blocking approximation give conflicting results for masses of odd nuclei. We systematically investigated the polarization and mean-field models, implemented within selfconsistent approaches that use identical interactions and model spaces, to find reasons for the conflicts between them. For

density-dependent interactions and with pairing correlations included, we derived and studied links between the mean-field and polarization results obtained for energies of odd nuclei. We also identified and discussed differences between the polarization-correction and full particle-vibration-coupling (PVC) models. Numerical calculations were performed for the mean-field ground-state properties of deformed odd nuclei and then compared to the polarization corrections determined using the approach that conserves spherical symmetry. We have identified and numerically evaluated self-interaction (SI) energies that are at the origin of different results obtained within the mean-field and polarization-correction approaches. Mean-field energies of odd nuclei are polluted by the SI energies, and this makes them different from those obtained using polarization-correction methods. A comparison of both approaches allowed for the identification and determination of the SI terms, which then can be calculated and removed from the mean-field results, giving the self-interaction-free energies.

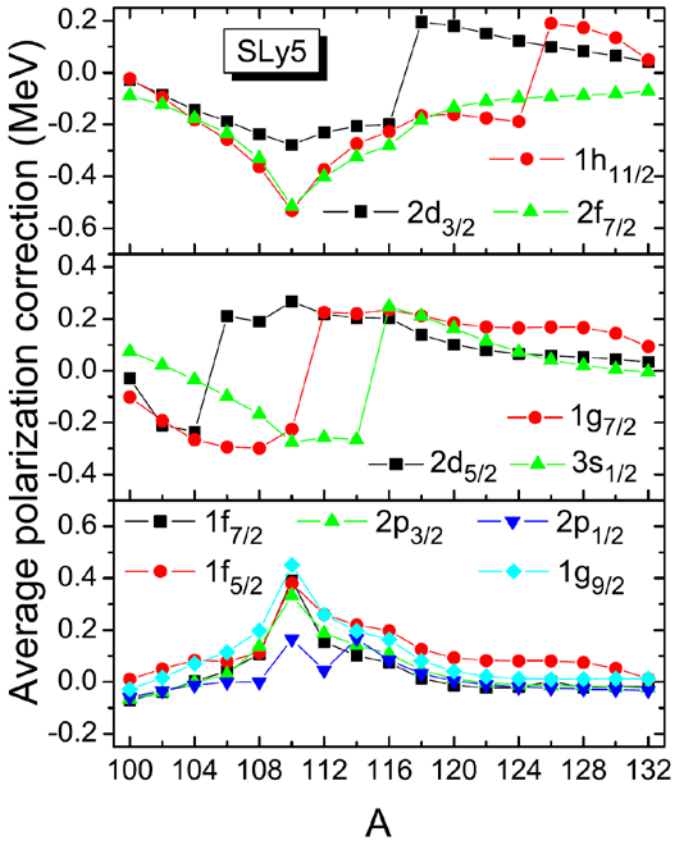

Fig. 2. Average QRPA (SIF + SI) polarization corrections in tin isotopes.

We addressed the question of how to improve the agreement between theoretical nuclear single-particle energies (SPEs) and observations. Empirically, in doubly magic nuclei, the SPEs can be deduced from spectroscopic properties of odd nuclei that have one more, or one less neutron or proton. Theoretically, bare SPEs, before being confronted with observations, must be corrected for the effects of the particle vibration coupling (PVC). We determined the PVC corrections in a fully self-consistent way. Then, we adjusted the SPEs, with PVC corrections included, to empirical data. In this way, the agreement with observations, on average, improved; nevertheless, large discrepancies still remained. We concluded that the main source of

disagreement is still in the underlying mean fields, and not in including or neglecting the PVC corrections. This work contains full tables of empirical and calculated results.

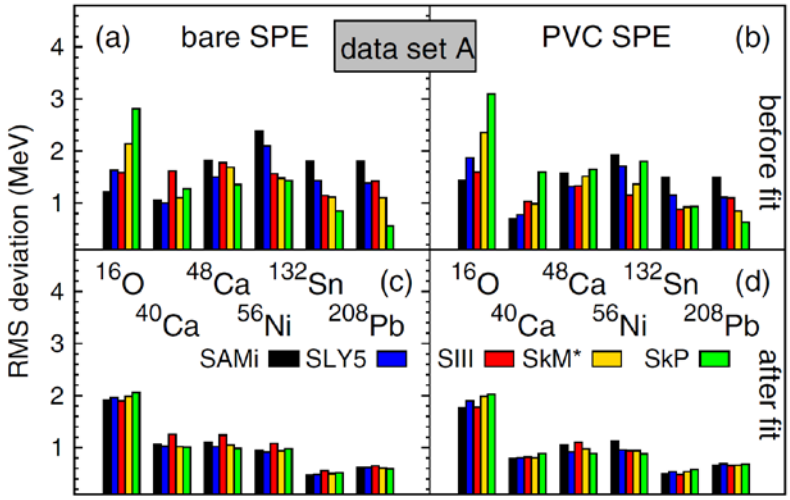

Fig. 3. Left (right) panels: root-mean-squared deviations between the bare (PVC-corrected) single-particle energies and empirical data of set A. Upper and lower panels show results obtained for standard Skyrme energy-density functionals and for refitted parametrizations, respectively. In all cases, partial contributions obtained in six doubly magic nuclei are shown.

Another aspect of the developments that we have realized concerns the introduction of correlations beyond a mean-field approach. The correlations that we have considered are those related to symmetry restorations, particle number and angular momentum, and to configuration mixing. These activities can be divided in two categories: applications to regions of the nuclear chart of special interest and new developments.

Applications have been done most often in collaboration with groups of experimentalists. We have studied in details the spectroscopic properties of nuclei in the region of the neutron deficient lead isotopes. These nuclei have a complicate structure and show several low-lying states that are interpreted as arising from the coexistence of two or three different shapes. Our calculations confirm this interpretation and are in general in good agreement with the experimental data. A typical result for three isotones is presented in Figure 4. Although the theoretical spectra are too spread, the main tendencies are well reproduced and the transition probabilities agree satisfactorily with the data. Note that no effective charges are introduced in the model. These calculations have generated a large set of results that are available to the community as supplementary material of a publication in Phys. Rev. C. This material has been used to support the publication of experimental data, especially of the determination of isotopic shifts.

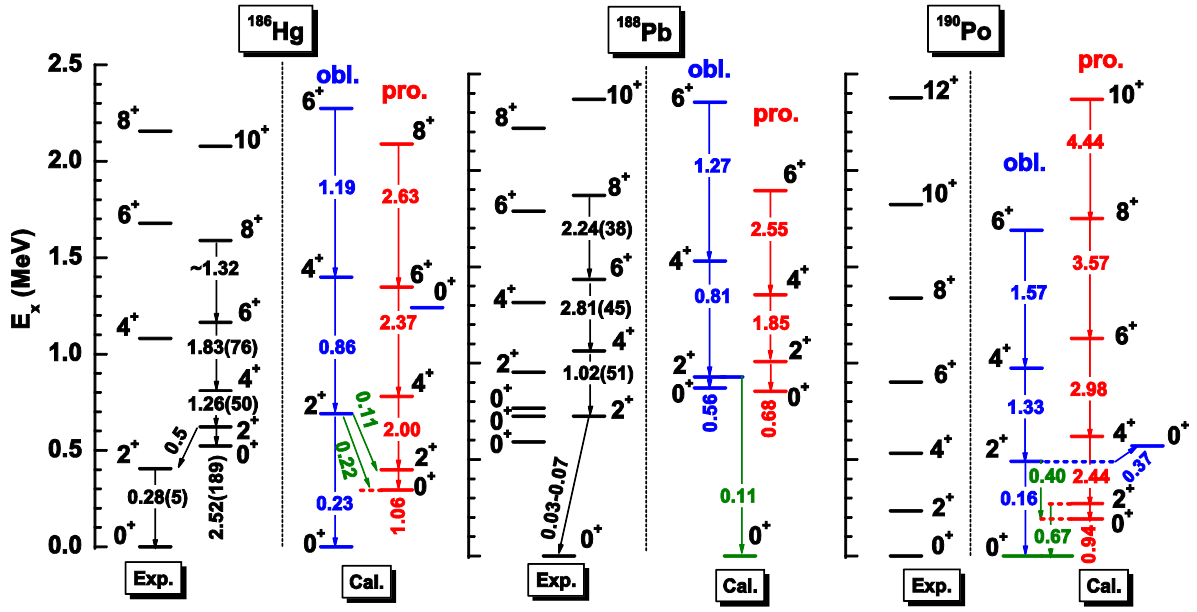

Fig. 4 Spectra of the N=106 isotones obtained using a beyond mean-field calculation, in comparison with the available experimental data.

Another systematic calculation has been performed for the Ni isotopes. In this case, the focus was on a new tool that we have developed to determine transition densities between low-lying states. Once again, this study has generated a large set of results on the spectra of these isotopes that have been made available to the community.

It has been demonstrated that pathologies can appear in beyond-mean-field calculations when some form of a density functional is used to model the nucleon-nucleon interaction. Forms that are safe in this respect have been developed in part within this project. Thanks to this and to new extensions of our model, as the inclusion of several quasi-particle excitations, it has then been possible to study nuclei with an odd number of neutrons or protons. A first application to 25Mg has demonstrated the potentialities of our model. The energies and the electromagnetic transition probabilities obtained for the ground state band of this Mg isotope are shown in Figure 5. The agreement with the data is very good and is obtained without fine tuning of the interaction and without the introduction of effective charges. This generalization of our model to odd nuclei but also to two quasi-particle states in even-even nuclei will greatly extend the potentialities of beyond-mean-field methods

Another extension of our model that has been undertaken during the ENSAR project is the generalization of the method to the description of left-right asymmetric shapes (the octupole degree of freedom). Several applications are close to completion, in particular the effect of correlations on fission barriers. We have demonstrated that the inclusion of projection on angular momentum reduces greatly the height of the fission barrier of 180Hg and brings it close to the experimental value.

Let us finally mention that the code Ev8, based on a discretization of the nucleon wave functions on a 3-dimensionnal Cartesian mesh has been published in a very detailed article. A special effort has been made to make this code user-friendly.

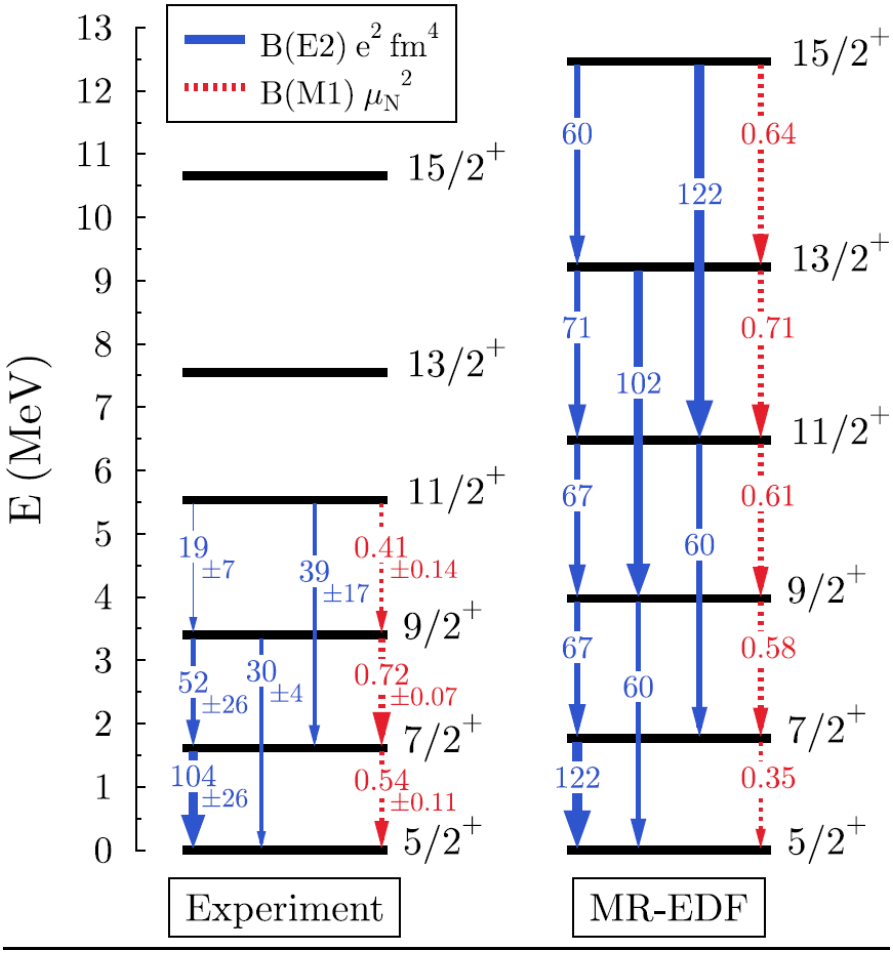

Fig. 5 Comparison between the spectrums obtained for 25Mg with our beyond-mean-field model (MR-EDF) and the experimental data.

List of publications of ENSAR/THEXO:

Solution of the Skyrme-Hartree-Fock-Bogolyubov equations in the Cartesian deformed harmonic-oscillator basis. (VII) HFODD (v2.49t): a new version of the program:
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submitted to JPS Conference Proceedings, arXiv:1407.0857.

Mean-field calculation based on proton-neutron mixed energy density functional :
K. Sato, J. Dobaczewski, T. Nakatsukasa, W. Satuła,
submitted to JPS Conference Proceedings, arXiv:1410.2691.

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Submitted to Phys. Rev. C