Vol. 12 (2019) *Acta Physica Polonica B Proceedings Supplement* No 3

EVOLUTION OF THE POSITION OF SINGLE-PARTICLE LEVELS IN NEUTRON-RICH CERIUM AND NEODYMIUM ISOTOPES* **

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(Received December 21, 2018)

Dedicated to the late Professor Adam Sobiczewski

Different Skyrme functional parametrizations were tested for Ce and Nd isotopes for $N > 82$. The method employed in the study is the axial Skyrme–Hartree–Fock model+BCS. For selected parametrizations, ground-state deformations β_2, β_3 and β_4 have been found and the evolution of single-neutron and single-proton states around the Fermi level along the chain of Ce and Nd isotopes has been investigated. These results were then compared to the existing experimental data.

DOI:10.5506/APhysPolBSupp.12.507

1. Introduction

Radioactive beam facilities at ORNL and RIKEN together with highly efficient arrays of HPGe detectors at neutron beam facilities (ILL) made the region of neutron-rich nuclei accessible for spectroscopic studies [1, 2]. To understand the structure of low-lying states in odd and odd–odd neutron-rich nuclei and to make the correct assignment of their spins and parities, a lot of experimental and theoretical effort has brought only a partial success, especially in the region around $A \sim 150$ [3–6].

* Presented at the XXV Nuclear Physics Workshop "Structure and Dynamics of Atomic Nuclei", Kazimierz Dolny, Poland, September 25–30, 2018.

** Supported by the project SP 2018/84. We thank Prof. P.-G. Reinhard for providing us with the Skyrme-HF + BCS code SKYAX.

Among the many methods used to study microscopic properties of nuclei, the nuclear density functional theory (DFT) plays a central role [7, 8]. A very high quality description of nuclear properties in different mass regions can now be reached using the Skyrme–Hartree–Fock (SHF), Gogny or the relativistic mean-field (RMF) versions of the DFT. An overwhelming majority of applications addresses even–even nuclei, the simplest nuclear systems to be studied. On the other hand, when aiming at single-particle spectra, for example, the data coming from odd-mass nuclei are needed. The theoretical description of odd nuclei is, however, far more complex than that of the even–even ones. In particular, time-odd mean fields (TOMF) that do not contribute to the ground state of non-rotating even–even nuclei, can be essential for a correct description of ground states of odd and odd–odd nuclei.

There have been very few systematic theoretical surveys of one-quasiparticle states in even–odd or odd–even nuclei. Macroscopic–microscopic approach has been used to obtain regional systematics of one-quasiparticle excitations and their impact on various observables in spherical and deformed nuclei [9–13], and nuclear DFT has been employed for a similar purpose in Refs. [14–16]. A global DFT study of ground-state spin and parity of odd-mass nuclei has been performed by Bonneau *et al.* [17]. It should be noted that all of these studies were restricted in some way (by assuming axial symmetry, neglecting TOMF *etc.*) and provided rather poor description of single-particle states. From the results of Refs. [17] and [18, 19], it was clear that evaluating of the magnitude of different theoretical restrictions was imperative.

Such a review was done in Ref. [20]. The authors have studied properties of odd–even and even–odd nuclei with $16 \leq Z \leq 92$ and the role played by the TOMF. The study reveals negligible TOMF effects for the spectra in comparison with the effects caused by various choices of the Skyrme parametrization. For all nuclear properties considered in their study, the best description was obtained with the recent parametrization SV-bas. Low-lying excitation spectra of odd nuclei next to doubly magic ones have been well described in some cases but not so well in others. It seems that the mismatch is probably caused by the coupling to vibrational degrees of freedom of the corresponding even–even cores. The effect of such a coupling could be particularly strong in deformed nuclei. A more detailed investigation of such correlations will be crucial for description of low-energy single-particle spectra of odd nuclei.

Another systematic theoretical survey of one-quasiproton states in deformed rare-earth nuclei including the effect of TOMF has been carried out in [21]. It has again been concluded that the contribution of TOMF to the energy of the ground state and low-lying excited states is very small (about 50 keV) and that more significant differences are found depending on the Skyrme parametrization employed. Among the three standard Skyrme parametrizations tested (SIII, SkP and Sly4), the SIII one gives the best reproduction of the experimental band heads for Ho isotopes. In general, the standard parametrizations of the Skyrme interaction gave a qualitative but not quantitative description of experimental one-quasiproton spectra in the rare-earth region; the general trends are well-reproduced and most of the Nilsson orbitals found experimentally are theoretically predicted in the neighborhood of the Fermi level, the quantitative agreement with the experiment is, however, less satisfactory. There are many factors that can impact the order of one-quasiparticle levels and a more detailed study to asses their importance is necessary.

Tarpanov *et al.* [22] have studied the polarization and mean-field models, implemented within self-consistent approaches that use identical interactions and model spaces, to find reasons for the conflicts between them. The RPA calculations have been performed with the density-independent Skyrme-SV [23] and SLy5 [24] functionals for the $^{100-132}$Sn nuclei. They have shown that mean-field energies of odd nuclei are polluted by the self-interaction energies, which makes them different from those obtained using polarization-correction methods. A procedure has been identified to subtract them from the mean-field results leading to self-energy-free masses.

Recently, deviations between calculated and measured band-head excitation energy spectra in well-deformed odd-mass heavy nuclei have been addressed in four odd-mass actinide, namely the ^{235}U, ^{239}Pu, ^{237}Np and ^{241}Am [25], using two effective interactions of the Skyrme type, namely the SIII [23] and SkM$*$ [26] parameter sets. The calculated spectra were in reasonable agreement with the available data for odd-neutron nuclei, while serious deviation from experiment has been found for odd-proton ones. The authors conclude that an explanation for such a difference in the quality of the evaluation of neutron-odd and proton-odd nuclei may be related to the use of the Slater approximation [27] to treat the Coulomb exchange approximation: The occupied states are unevenly shifted upwards and the unoccupied states downwards, which perturbs in an uncontrolled fashion the relative ordering of nuclear levels. To assess the effect of this approximation on the odd-proton nuclear spectra, a significant numerical effort will be needed in the future calculations.

The importance of a correct treatment of the particle-vibration coupling (PVC) for a proper description of the odd nucleus has been stressed in many works (*e.g.* in studies of single-particle states around a magic core by using PVC based on the Skyrme Hamiltonian [28–30]). However, the low-lying spectra of odd nuclei are characterized by the simultaneous presence of states having quite different physical nature. A first step to generalize the concept of PVC calculations, in a nonperturbative way, for the case of odd nuclei ^{49}Ca and ^{133}Sb made up with a particle around a magic core, has been done in Ref. [31]. Single-particle states from HF calculations were coupled noafant only with genuine vibrations of the core but with all the excitations emerging from RPA calculations that include both collective and noncollective states. The model has well accounted for the ordering and the absolute energy of the low-lying states with an impressive precision. Some discrepancies, however, still persist, which call for further improvement of the model (*e.g.* including both the interaction between the particle plus core excitation states, and the contribution of more complicated configurations).

In the contribution, after a brief description of SHF model in Sect. 2, we present results of tests of different Skyrme functional parametrisations and found ground-state deformations (β_2, β_3, and β_4) for neutron-rich even–even Ce and Nd isotopes with $N \geq 82$ in Sect. 3. For selected parametrizations, the evolution of single-neutron and single-proton states around the Fermi level along the two isotopic chains has been then investigated and the results compared to existing experimental data from odd-Ce, odd-Pr, odd-Nd and odd-Pm nuclei.

2. Skyrme density functional with BCS pairing

The Skyrme energy density functional (SDF) $\mathcal{H}_{\mathrm{Sk}}[J_d(\vec{r})]$ depends on a set of densities $J_d(\vec{r})$ [7]. The Hartree–Fock (HF) Hamiltonian $\hat{H}$ can be heuristically obtained by variation with up to first-order functional derivatives

$$\hat{H} = \sum_i \varepsilon_i \hat{\alpha}_i^\dagger \hat{\alpha}_i = \sum_d \int \frac{\delta \mathcal{H}_{\mathrm{Sk}}}{\delta J_d(\vec{r})} \hat{J}_d(\vec{r})\, \mathrm{d}\vec{r}, \tag{1}$$

where the single-quasiparticle energies ε_i are from HF+BCS. In calculations using the axial Skyrme–HF code SKYAX with a density-dependent δ-force interaction in the pairing channel [32], two model spaces were tested, a smaller one comprising ~ 10 oscillator shells, and a larger one comprising ~ 22 oscillator shells. There are plenty of SHF functional parametrizations available in the literature. Here, we refer to a recent family of parametrizations derived from least-square fitting of its free parameters to a large pool of selected g.s. observables and other nuclear properties over the whole nuclear chart (incompressibility, symmetry energy, effective isoscalar and isovector masses) [33]. We have checked for the present test cases all 15 of them and in additions 6 older choices, namely Sk-M*, SLy4, SLy5, SLy6, SkI3, and SIII reported in Ref. [21] to reproduce the g.s. spins and parities of odd-proton rare earth nuclei quite correctly.

3. Results and conclusions

In Fig. 1, the evolution of the potential energy curves (PEC) as a function of the quadrupole deformation parameter β_2 in the chains of Ce and Nd isotopes for the parametrization SV-bas (base point for dedicated variation of nuclear matter properties in [33] and giving the best description of properties of odd nuclei in [20]) for the smaller model space is shown. We

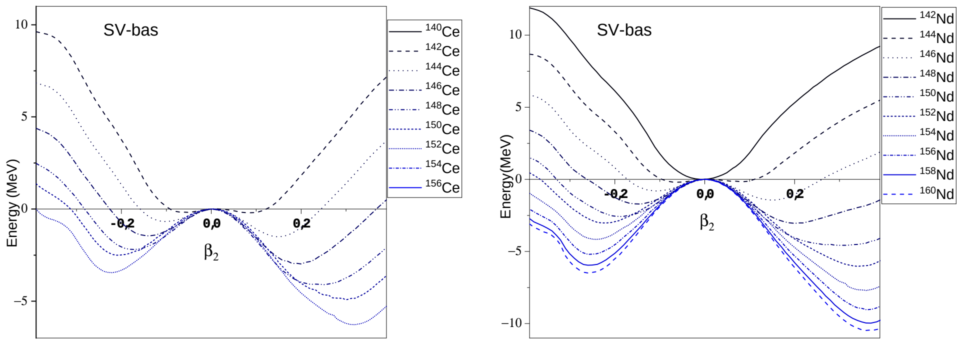

Fig. 1. PEC for a chain of Ce (left) and Nd (right) isotopes as a function of β_2 for the SV-bas parametrization.

start at spherical nuclei, ^{140}Ce and ^{142}Nd, continue through the transitional region where the oblate and prolate minima are not well-separated in energy, and end in the deformed region with one pronounced prolate minimum ($^{150-158}$Ce and $^{152-160}$Nd). In this region, the octupole correlations do not play a significant role as can be seen in Fig. 2. The other parametrizations give similar qualitative behavior. For the larger model space, the PEC minima are slightly shifted, but again the similar qualitative behavior is obtained.

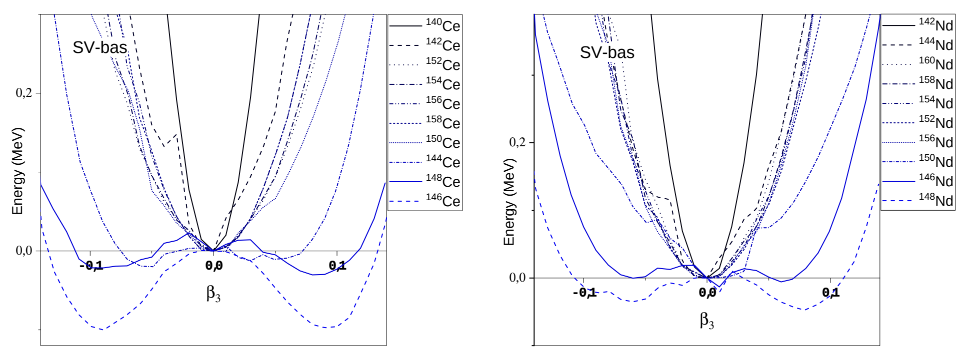

Fig. 2. PEC for a chain of Ce (left) and Nd (right) isotopes as a function of β_3 for the SV-bas parametrization.

In the above-mentioned region with the one pronounced prolate minimum, large amplitude correlations can be neglected and the evolution of single-particle neutron and proton states along the chains of Ce, Pr, Nd and Pm isotopes can be investigated for the g.s. energy minimizing sets of β_2 and β_4 deformation parameters. The results for the smaller model space and the SLy6 parametrization are shown in Figs. 3–4.

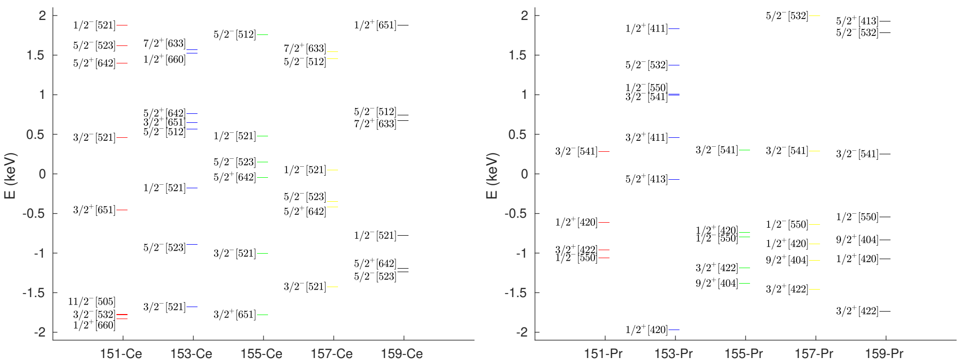

Fig. 3. Evolution of single-particle neutron (left) and proton (right) states (dominant Nilsson configurations are indicated) for the chains of Ce and Pr isotopes for the SLy6 parametrization and the smaller model space. The Fermi energy of the even–even core is set to be 0 MeV.

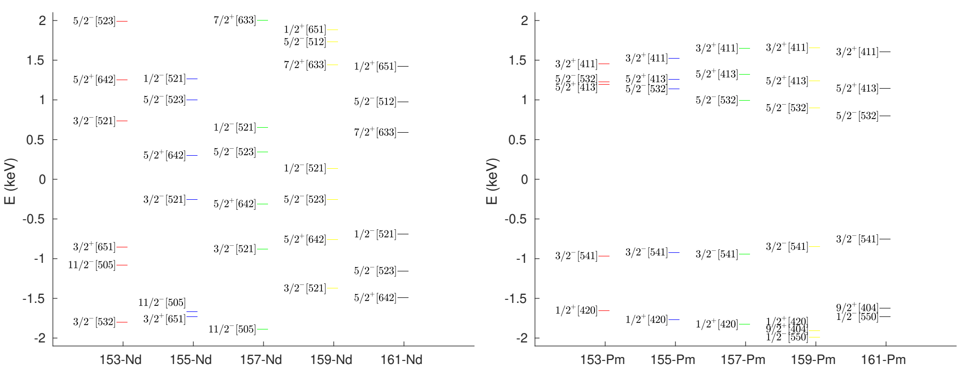

Fig. 4. The same as in Fig. 3, but for the chains of Nd and Pm isotopes.

Assignments of the experimentally observed levels in the studied region are mostly tentative and rather scarce [34]. For the majority of nuclei, only ground states are assigned. The exceptions are ^{153}Pm (4 assigned Nilsson configurations), ^{153}Nd and ^{155}Pm (2 assigned Nilsson configurations). For ^{151}Ce, the adopted evaluated g.s. configuration ($5/2^+[642]$ [35]) differs from the recently proposed assignment $3/2^-[521]$ [36].

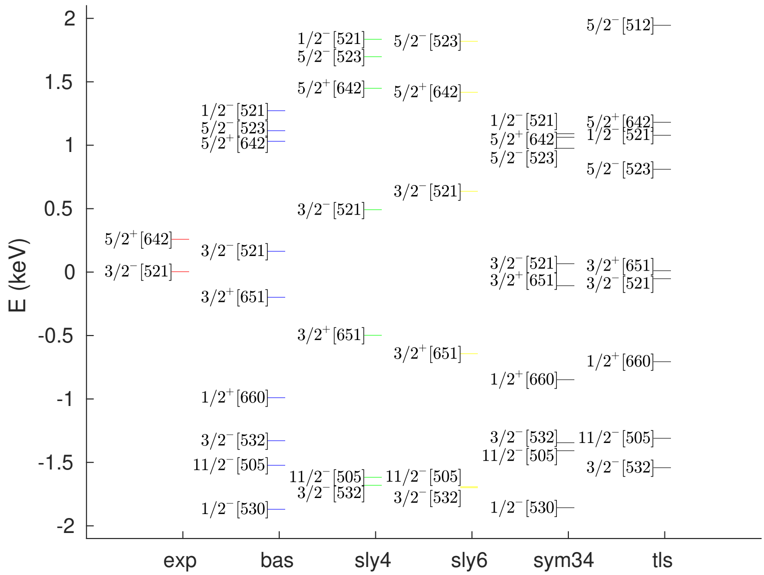

Fig. 5. Low-lying single particle neutron configurations in ^{151}Ce calculated for the larger model space and different parametrizations compared to experimental data [36].

The parametrization SLy6 seems to fit best the g.s. spins and parities and assigned excited bandheads (only for ^{153}Nd the predicted energy of the $5/2^-[523]$ configuration lies to high and the parametrization tls that best fits the g.s. binding energies of even–even Ce and Nd isotopes gives a better result for the large model space, and the tentatively assigned g.s. configurations of ^{153,157}Ce, ^{153}Pr and ^{159,161}Nd are not reproduced). The family of parametrizations based on SV-bas fails to reproduce the $5/2^-[532]$ ground state for ^{153}Pm in the smaller model space. In the larger model space, it predicts the correct g.s. configuration but fails in reproducing the spacing between the two lowest configurations ($5/2^-[532]$, $5/2^+[413]$) and the $3/2^+[411]$ (the calculated values are almost degenerated, whereas experimentally $3/2^+[411]$ lies about 0.45 MeV above $5/2^-[532]$ and $5/2^+[413]$). For ^{151}Ce, all parametrizations favour $3/2^-[521]$ as the g.s. configuration in agreement with the recent experimental data [36] (*cf.* Fig. 5).

To conclude, we recommend using the SLy6 parametrization for calculations of single-particle proton and neutron levels in odd-A Ce, Pr, Nd and Pm isotopes and, for future calculations, taking into account couplings between single-particle, vibrational and rotational degrees of freedom.

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