Contrasting properties of particle-particle and hole-hole excitations in ^{206}Tl and ^{210}Bi nuclei

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ABSTRACT

A complete-spectroscopy investigation of low-lying, low-spin states in the one-proton-hole and one-neutron-hole nucleus ^{206}Tl has been performed by using thermal neutron capture and γ-coincidence technique with the FIPPS Ge array at ILL Grenoble. The new experimental results, together with data for the one-proton-particle and one-neutron-particle nucleus ^{210}Bi (taken from a previous study done at ILL in the EXILL campaign), allowed for an extensive comparison with predictions of shell-model calculations performed with realistic interactions. No phenomenological adjustments were introduced in the calculations. In ^{210}Bi, state energies, transition multipolarities and decay branchings agree well with theory for the three well separated multiplets of states which dominate the low-lying excitations. On the contrary, in ^{206}Tl significant discrepancies are observed: in the same energy region, six multiplets were identified, with a significant mixing among them being predicted, as a consequence of the smaller energy separation between the active orbitals. The discrepancies in ^{206}Tl are attributed to the larger uncertainties in the determination of the off-diagonal matrix elements of the realistic shell-model interaction with respect to the calculated diagonal matrix elements, the only ones playing a major role in the case of ^{210}Bi. The work points to the need of more advanced approaches in the construction of the realistic interactions.

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Odd-odd two-valence-particles/holes systems around the most magic of all nuclei, ^{132}Sn and ^{208}Pb, are ideal to test advanced shell-model approaches. Unfortunately, the one-proton-hole and one-neutron-hole nucleus ^{130}In and the one-proton-particle and one-neutron-particle nucleus ^{134}Sb are difficult to reach for spectroscopic studies. On the contrary, the accessibility of low-lying excitations in the corresponding (with respect to the ^{208}Pb core) ^{206}Tl and ^{210}Bi nuclei, in neutron capture and transfer reactions with stable beams, make them unique systems to benchmark the proton-neutron shell-model interactions derived from the bare nucleon-nucleon potential.

In this work, we aim at obtaining experimental results on the low-energy structures in ^{206}Tl populated in thermal neutron capture reaction and, together with existing similar data on the ^{210}Bi nucleus, compare them to theoretical predictions using shell-model calculations based on effective interactions derived from the realistic nucleon-nucleon CD-Bonn potential. For the first time, not only energy spectra, but also decay branchings were considered. A detailed comparison of the experimental excitation energies of ^{210}Bi with shell-model results is reported in Ref. [1], where calculations were performed by employing the pioneering realistic interaction developed by Kuo-Herling [2] with the empirical modifications introduced in Ref. [3] and later works. Here, we intend to ascertain the reliability of modern realistic effective interactions in the description of the low-lying excitations of nuclei around ^{208}Pb, without introducing any phenomenological adjustments, so to better evaluate their predictive power. The results we obtain
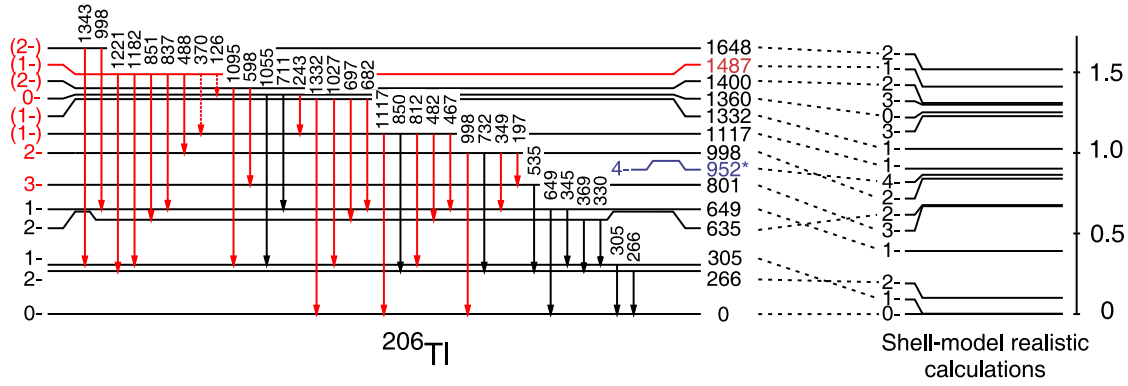

Fig. 1. Partial level scheme (up to 1.5 MeV) of ^{206}Tl populated in the thermal neutron capture reaction on ^{205}Tl (left), compared to shell-model realistic calculations (right). The 4$^-$ level, not observed in the present data, is marked by an asterisk.
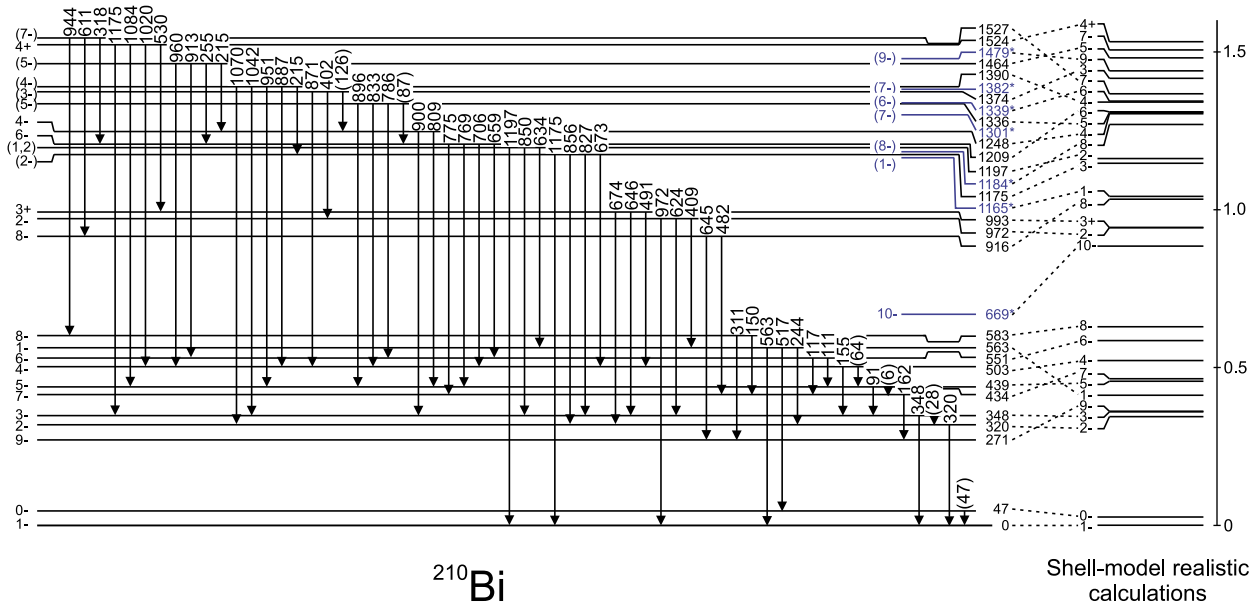

Fig. 2. The partial level scheme (up to 1.5 MeV) of ^{210}Bi populated in the thermal neutron capture reaction on ^{209}Bi (left) [1] compared to the shell-model realistic calculations discussed in this work (right). The (10$^-$), (1$^-$), (8$^-$), (7$^-$), (6$^-$), (7$^-$), (9$^-$) levels, not observed in the work of Ref. [1], are marked by the asterisks.

for ^{210}Bi, with two-valence particles outside ^{208}Pb, have been, in part, presented in Ref. [4]. There, it was shown that our effective interaction is able to reproduce remarkably well the lowest-lying multiplet and in particular to predict the correct ground-state spin, $J^\pi = 1^-$, as arising from core-polarization effects induced by the nucleon-nucleon potential – they are responsible for the inversion of the 1$^-$ and 0$^-$ states. In the present paper, we extend the comparison between theory and experiment for ^{210}Bi by considering higher-lying states and decay branchings, and we also report results for ^{206}Tl, with two-valence holes with respect to ^{208}Pb. We shall see that while in ^{210}Bi, state energies, transition multipolarities and decay branchings agree well with theory, in the case of ^{206}Tl significant discrepancies are observed. They are attributed to larger uncertainties in the determination of the off-diagonal matrix elements of the realistic shell-model interaction with respect to the calculated diagonal matrix elements, which play the major role in the case of ^{210}Bi.

In ^{206}Tl, almost all states (12 out of 13 reported in this paper) up to 1.5 MeV excitation energy were observed in transfer reactions, beta-decay and previous thermal neutron capture studies, and were interpreted as members of six multiplets involving the proton $s_{1/2}$, $d_{3/2}$ and neutron $p_{1/2}$, $p_{3/2}$ and $f_{5/2}$ orbitals [5] (see

Fig. 1). However, information on γ decays and spin-parity assignments was largely missing. On the contrary, complete spectroscopy of ^{210}Bi was recently achieved in a cold neutron capture study carried out at ILL, during the EXILL campaign [1,6]. Here, in the excitation energy region below 1.5 MeV, 21 states have been located (15 with firm spin-parity assignments) and their γ-decay pattern has been established, as shown in Fig. 2. In this case, all negative parity states (20 in total) belong to the lowest three multiplets $\pi h_{9/2} \nu g_{9/2}$, $\pi h_{9/2} \nu i_{11/2}$ and $\pi f_{7/2} \nu g_{9/2}$.

The ^{206}Tl and ^{210}Bi isotopes were investigated in two separate neutron-capture experiments, performed at Institut Laue-Langevin (ILL) in Grenoble, France.

The coincidence measurements of γ rays from the thermal-neutron capture on ^{205}Tl were performed with the newly constructed detection system – FIPPS (FIssion Product Prompt gamma-ray Spectrometer) [7]. FIPPS is an array consisting of 8 HPGe clovers (for a total of 32 HPGe crystals), arranged in annular geometry at every 45° around the target, which was in this case a sample of 99.9% enriched ^{205}Tl isotope, with total weight of ∼2 g. Digital electronics was used to collect and process the signals from the detectors. Each event contained information on γ-ray energy, time and identification number of the specific crystal that
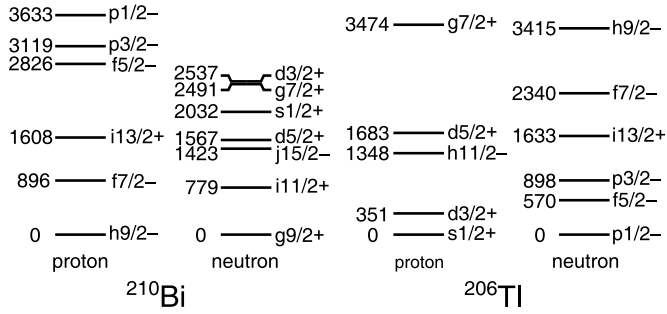
Fig. 3. Single-particle and single-hole states adopted for the ^{210}Bi and ^{206}Tl shell-model calculations, discussed in this work.

fired. The data were stored triggerless and sorted offline into a $\gamma\gamma$-coincidence matrix and a cube [8].

A total number of 22 primary γ rays (10 new) from the capture state was observed in ^{206}Tl. They populate 21 excited states, 8 of which are reported for the first time. The full γ-decay scheme from the capture state and the analysis of the γ-ray angular correlations will be discussed in Ref. [9], while preliminary results, including the coincidence spectra, have been already presented in [10]. In this paper, we would like to discuss only the states up to 1.6 MeV in the ^{206}Tl isotope, as presented in Fig. 1. They arise from the couplings between one-valence-proton-hole and one-valence-neutron-hole excitations. As the γ decay originates from the capture state, which in this case may have 0^+ or 1^+ spin-parity values, only very low-spin excitations, with spins from 0 to 3, were populated. The γ-angular correlation analysis of the present data allowed to firmly establish the spins of the 801-, 998-, and 1360-keV states as 3^-, 2^-, and 0^-, respectively. Moreover, this analysis helped to assign the spin-parity values for the 1117-, 1332-, and 1648-keV excitations as (1^-), (1^-), and (2^-), which were previously reported as $(1^-,2^-)$. Furthermore, the spin value (2^-) was here proposed to the excitation at 1400 keV, the γ decay of which was previously not reported. Among the considered states, the excitation at 1487 keV with $J^\pi = (1^-)$ was newly established. We note that this may be the same state as the one which was reported in NNDC at 1490 keV. Further, the presence of the levels placed at 939, 1080, 1206, 1453, and 1631 in the previous neutron capture experiment [11,12] was not confirmed.

In ^{210}Bi, states with spins from 0 to 9 were studied in the cold-neutron-capture reaction with the EXILL setup described in Ref. [13]. In that work, 64 primary γ rays from the capture state were observed: they populate 70 discrete states, 33 of which were newly identified. Details of the experiment and of the analysis are described in Refs. [1,6], where a comparison with shell-model calculations based on phenomenological interactions is also presented. In this work, we focus on the lower lying levels (up to 1.5 MeV) in ^{210}Bi, as shown in Fig. 2, originating only from the couplings between one-valence-proton and one-valence-neutron excitations.

Shell-model calculations have been performed for ^{210}Bi and ^{206}Tl using a realistic two-body effective interaction. As model space, we have considered one proton major shell and one neutron major shell above and below ^{208}Pb, respectively, for ^{210}Bi and ^{206}Tl. The adopted spaces are shown in Fig. 3, where we also report the single-particle and single-hole neutron and proton energies, that are taken from the experimental spectra of one-valence particle/hole nuclei, namely from ^{209}Pb and ^{209}Bi for ^{210}Bi and ^{207}Pb and ^{207}Tl for ^{206}Tl [5].

The neutron-proton matrix elements of the Hamiltonian have been derived by using the perturbative many body theory [14] within the particle-particle formalism for ^{210}Bi, and the hole-hole
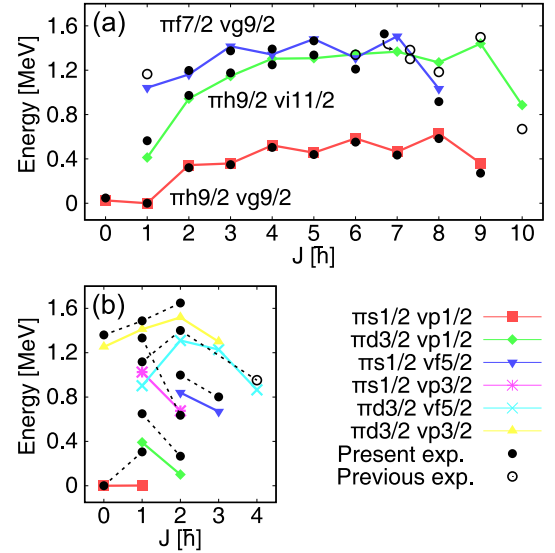

Fig. 4. (a) The three lowest lying multiplets of ^{210}Bi below 1.5 MeV excitation energy, calculated and measured in the thermal neutron capture reaction on ^{209}Bi (full circles) or other reactions (open circles). The 7^- state, located in our previous work at 1527 keV [1], belongs to the second multiplet ($\pi h_{9/2} \nu i_{11/2}$), as suggested by the branching ratios (see text). (b) The six lowest lying multiplets of ^{206}Tl below 1.6 MeV excitation energy, calculated and measured in the thermal neutron capture reaction on ^{205}Tl (full circles) or other reactions (open circle).

one for ^{206}Tl. We start from the realistic CD-Bonn free nucleon-nucleon potential [15] and use the $V_{\mathrm{low}-k}$ approach [16], with a cutoff momentum = 2.2 fm^{-1}, to integrate out its high-momentum components. Then, the smooth $V_{\mathrm{low}-k}$ potential is used within the $\hat{Q}$-box folded diagram expansion, including all diagrams up to second order in $V_{\mathrm{low}-k}$, to derive the effective shell-model interaction. In this way, the bare matrix elements of the nucleon-nucleon potential are renormalized to take into account the contributions arising from the neutron and proton excitations across the 126 and 82 shells. More details on the derivation of the effective interaction used for ^{210}Bi can be found in [4].

Experimental and calculated levels of ^{210}Bi are compared in Fig. 2 (the 10^- state, not observed in the (n,γ) experiment of Ref. [1], is taken from Ref. [5]). We see that experimental energies are satisfactorily reproduced by theory – state energy differences between theory and experiment range from a few keV to a maximum of $\sim$200 keV for the 10^- state at 669 keV, with a standard deviation of 80 keV only. In particular, the calculations correctly reproduce the 1^- experimental ground state, which was a long-standing problem, as discussed in [4].

Up to about 1.5 MeV excitation energy, three long multiplets can be identified in ^{210}Bi, as shown in Fig. 4(a). These multiplets, that exhibit the typical downward parabolic behavior, arise from the $\pi 0 h_{9/2} \nu 0 g_{9/2}$, $\pi 0 h_{9/2} \nu 0 i_{11/2}$, and $\pi 1 f_{7/2} \nu 0 g_{9/2}$ configurations. The members of the lowest-lying multiplet are almost pure – the $\pi 0 h_{9/2} \nu 0 g_{9/2}$ configuration contribution is >91%. Members of the other two multiplets are instead characterized by some admixtures, which are particularly relevant for the $1^-_{2,3}$, $2^-_{2,3}$, and $6^-_{2,3}$ states, where dominant components range from 52 to 61%. The percentages of the various configurations for the states of ^{210}Bi are shown in panels (g)-(i) of Fig. 5. No states arising from higher energy multiplets appear below 1.5 MeV, except for the lowest-spin member, 3^+, of the $\pi 0 h_{9/2} \nu 0 j_{15/2}$ configuration, that having positive parity cannot admix with the states of the three lowest-lying multiplets. It is worth mentioning, that a good overall agreement between the calculated and experimental spectra of ^{210}Bi – with a standard deviation of about 150 keV – was also obtained in Ref. [3]
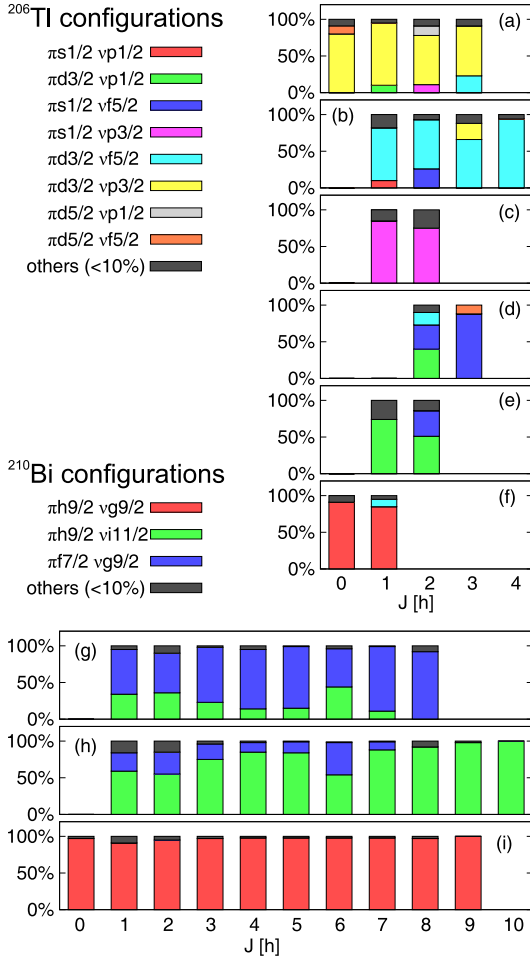
206Tl configurations

πs1/2 νp1/2
πd3/2 νp1/2
πs1/2 νf5/2
πs1/2 νp3/2
πd3/2 νf5/2
πd3/2 νp3/2
πd5/2 νp1/2
πd5/2 νf5/2
others (<10%)

210Bi configurations

πh9/2 νg9/2
πh9/2 νi11/2
πf7/2 νg9/2
others (<10%)

Fig. 5. Percentage of the main configurations (> 10%) in the six lowest multiplets calculated for ²⁰⁶Tl (a)-(f) and the three lowest multiplets calculated for ²¹⁰Bi (g)-(i).

Fig. 6. Comparison between experimental and calculated branching ratios in ²¹⁰Bi and ²⁰⁶Tl.

by using the Kuo-Herling interaction with only the bare and core-polarization contributions, the latter being scaled by a factor of 0.92. However, to reproduce the inversion of the 1^- and 0^- states and to improve, in general, the agreement with experiment, other modifications of the Kuo-Herling interaction were proposed by varying selected two-body matrix elements, as done in [3] and later works. The spectrum resulting from this phenomenologically-adjusted interaction, shown in Ref. [1], has a very good agreement with the experiment for the states which were used in the fitting procedure while for other excitations the agreement is similar to the one obtained in the present calculations.

Experimental and calculated excitation energies for ²⁰⁶Tl are compared in Fig. 1. In this case, agreement between experiment and theory is not as good as for ²¹⁰Bi. Discrepancies between experimental energies and calculated levels range from ∼40 to 300 keV, and the standard deviation increases to 180 keV, with discrepancies larger than 200 keV for the four lowest-lying 1^- states. As in previous shell-model calculations [17,18], we find a $J = 1$ state almost degenerated with the 0^- ground state, while experimentally the 0^- ground state is well separated from the 1^- yrast state.

By looking at the compositions of the wave functions for ²⁰⁶Tl, we can identify four doublets and two multiplets below 1.5 MeV, which are reported in Fig. 4(b). As shown in panels (a)-(f) of Fig. 5, their members are characterized by a significant configuration mixing, namely they receive sizable contributions from configurations other than the dominant one.
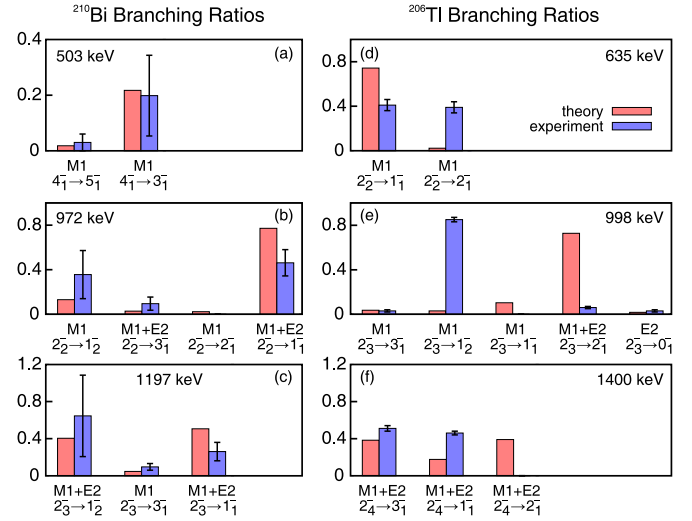
The more complex structure observed in ²⁰⁶Tl with respect to that of ²¹⁰Bi, arises from the different features of the shell-model orbitals which are active in the two cases.

Considering the single-particle energy spectrum of ²¹⁰Bi (see Fig. 3 left), the unperturbed energies of the three lowest-lying multiplets, reported in Fig. 4(a), are separated by ∼700 keV from the higher-lying negative-parity $\pi 0h_{9/2} \nu 2d_{5/2}$ multiplet, and a significant gap of ∼700 keV exists between the lowest-lying and the next two multiplets. Such multiplets are, therefore, scarcely affected by the off-diagonal matrix elements of the two-body interaction, whose values are not larger than 300 keV, most of them being of the order of a few tens of keV. A non-negligible admixture is found for the $\pi 0h_{9/2} \nu 0i_{11/2}$, and $\pi 1f_{7/2} \nu 0g_{9/2}$ configurations only.

In the case of ²⁰⁶Tl, the energy gaps between the unperturbed first 6 low-lying multiplets shown in Fig. 4(b) (see Fig. 3 right) range from 200 to 300 keV, and the next negative-parity configuration, $\pi 2d_{5/2} \nu 2p_{1/2}$, lies only 400 keV above. As a consequence, the eigenvalues and the composition of the states in ²⁰⁶Tl are very sensitive to the off-diagonal matrix elements of the two-body interaction. Therefore, a fine tuning of the latter would be needed to improve the agreement with experiment.

To gain further insight into the structure of the states of both nuclei, we have considered the decay branchings, which may provide information on the wave function fragmentation. In Fig. 6, experimental and calculated branching ratios for ²¹⁰Bi and ²⁰⁶Tl are compared in a few selected cases which are representative of the multiplets discussed above. A more extended comparison will be given in Ref. [9].

Panels on the left show the decay branchings for the 4_1^-, 2_2^- and 2_3^- states of ²¹⁰Bi, while panels on the right refer to the 2_2^-, 2_3^- and 2_4^- states of ²⁰⁶Tl. As observed for the excitation energies, the quality of the agreement between theory and experiment is very good in ²¹⁰Bi. This result makes us confident that calculated branching ratios can help assessing spin-parity assignments of the lowest lying states in ²¹⁰Bi. In this way, firm spin-parity assignment of 3^-, 2^- and 3^- could be made to the levels located experimentally at 1175, 1197, and 1374 keV, respectively (previous assignments were: (2^-), $(1,2)$, and (3^-)), having their theoretical counterparts at 1147 keV, 1162 keV (cf. Fig. 6(c)), and 1416 keV. The 1165-keV state, observed in the past in a neutron-capture measurement [19] and assigned as 1^-, was not observed in our data but it was added for completeness.

Furthermore, four experimental 7^- states are proposed in literature in the energy region up to 1.5 MeV, while theoretical calculations predict only three excitations with such spin. Based on branching ratios comparison, the 7^- excitations at 434 and 1527 keV, observed in our work of Ref. [1], are here assigned to the theoretical 7_1^- and 7_2^- levels at 464 and 1367 keV, respectively. Out of the two other states with tentative (7^-) spin-parity assignments, located at 1301 and 1382 keV excitation energies in older works (but not confirmed in Ref. [1]), one could correspond to the theoretical 7_3^- level calculated at 1506 keV, although no sufficient information is available to firmly establish this correspondence. All four 7^- states are presented in Fig. 4(a).

Turning now to ^{206}Tl, the states wave functions, as mentioned above, are found to be highly fragmented, with admixture of various configurations. This makes the ^{206}Tl nucleus an ideal case for an extended test of the quality of the two-body effective interaction, with emphasis on the non-diagonal matrix elements. As seen in Fig. 6(d)-(f), pronounced differences are found between experimental and theoretical branching ratios, qualitatively much larger than the deviations observed for state energies. For example, in the case of the 2_3^- located at 998 keV (predicted by theory 158 keV below), the strongest experimental branch is the M1 decay to the 1_2^- state at 649 keV, while a strong M1 branch to the 2_1^- state is expected. The comparison between experiment and shell-model calculations with state-of-the-art realistic interactions for the two very simple systems ^{206}T and ^{210}Bi reveals limitations in the procedure of the off-diagonal matrix elements determination, the latter being responsible for the configuration mixing. An improvement in the determination of the non-diagonal matrix elements of the shell-model interaction is therefore needed in order to increase the reliability of our calculations.

To conclude, predictions of shell-model calculations, performed with realistic interactions, without introducing any phenomenological adjustments, were tested on ^{210}Bi and ^{206}Tl nuclei, which are unique systems to benchmark proton-neutron interactions in the particle-particle and hole-hole spaces, with respect to the doubly magic ^{208}Pb core. Experimental low-lying, low-spin states, populated in neutron capture reactions at ILL (Grenoble), allowed for an extensive comparison with theory. For the first time, not only states energies, but also γ branching ratios were considered, resulting in a rather stringent test of the shell-model wave functions calculated with realistic interactions.

Striking differences are found between ^{210}Bi and ^{206}Tl. In the case of ^{210}Bi, state energies, transition multipolarities and decay branchings for all states below 1.5 MeV (belonging to three rather pure multiplets) are very well reproduced by theory. In contrast, in the ^{206}Tl nucleus much larger discrepancies between theory and experiment are seen considering the 6 low-lying multiplets identified in the same 1.5-MeV interval. The ^{206}Tl multiplets are significantly mixed, as a consequence of the smaller energy separation between the active orbitals. Therefore, the observed discrepancies are attributed to the larger uncertainties in the determination of the off-diagonal matrix elements of the realistic shell-model interaction, which play a key role in the fragmentation of the state wave functions.

The work clearly points to the need of more advanced approaches in the construction of realistic interactions, which turn out to be remarkably uncertain already in the proximity of the valley of stability. Similar studies in exotic regions of the nuclear chart, as for example around doubly magic ^{132}Sn, would represent a major step forward in our basic understanding of nuclear forces in the nuclear medium.

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