The structure of tin isotopes with a global optimized effective interaction

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Abstract. A systematic shell model calculation on the structure of light tin isotopes is presented with a monopole-optimized effective interaction. We started with the realistic CD-Bonn potential. The unknown single-particle energies and the $T = 1$ monopole interactions are determined by fitting to the binding energies of the yrast states of nuclei $^{102\text{–}132}\text{Sn}$. The mean deviation from experimental data is around 120 keV. In particular, we analyzed the origin of the spin inversion between $^{101}\text{Sn}$ and $^{103}\text{Sn}$.

In this contribution I present a systematic study on the structure of light tin isotopes. We apply the so-called nuclear shell model. It should be mentioned that the term “shell model” is somewhat confusing since it is more often referred to the independent particle model proposed by Mayer and Jensen. The present shell model may be more precisely described as a full configuration interaction approach. It constructs the wave function as a linear expansion of all possible anti-symmetric Slater determinants within a given model space (Hibert space). In nuclear physics the model space is usually defined by taking into account the single-particle orbits between two adjacent magic numbers. On the first glance one may say that this truncation is a rather coarse approximation. But it works astonishingly well in most nuclei that have been studied. The present work is based on a paper we published recently [1].

The light tin isotopes between shell closures $N = 50$ and 82 are the longest chain that can be reached by contemporary shell model calculations. It is well established that the excitation energies of the first $2^+$ states in even-$A$ tin isotopes possess an almost constant value [2], which can be explained from the simple generalized seniority scheme [3]. A realistic description of these nuclei requires a knowledge of the effective interaction between the valence nucleons [4]. Shell model calculations have been very successful in explaining the structure and decay properties of light nuclei below $^{100}\text{Sn}$ (see, e.g., Refs. [4, 5, 6, 7] and references therein). The key to these calculations is a proper description of the monopole channel of the effective interaction which determines its bulk properties. Extensive shell-model calculations suggest that the realistic interaction can give a satisfactory description of the multipole part but not the monopole channel, which may be due to the lack of three-body forces [8, 9]. Thus we are motivated to fine-tune the monopole part of the realistic interaction by fitting to available experimental data in tin isotopes. We expect that the refined effective Hamiltonian will give a better understanding of the structure of trans-tin nuclei [1, 10, 11, 12, 13].

We assumed the doubly-magic nucleus $^{100}\text{Sn}$ as the core. For the model space we choose the neutron and proton orbitals between the shell closures $N = Z = 50$ and 82, comprising $0g_{7/2}$, $1d_{5/2}$, $1d_{3/2}$, $2s_{1/2}$ and $0h_{11/2}$. We also assume isospin symmetry in the effective Hamiltonian.
The monopole interaction is defined as the angular-momentum-weighted average value of the diagonal matrix elements $\langle j_\alpha j_\beta | V | j_\alpha j_\beta \rangle_{JT}$ for a given set of $j_\alpha$, $j_\beta$ and $T$. For the chosen model space there are 15 $T = 1$ monopole terms. The single-particle energies are assumed to be the same for all nuclei within the model space. They are given relative to the neutron $0g_{7/2}$ state. The energy of the $1d_{5/2}$ is taken as $\varepsilon(1d_{5/2}) = 0.172$ MeV [14]. The energies of other states are adjusted to fit the experimental binding energies of tin isotopes. The starting point of our calculation is the realistic CD-Bonn nucleon-nucleon potential which was renormalized using the perturbative G-matrix approach [4]. To minimize the $\chi^2$ function we apply a Monte Carlo global optimization (MC) method which we developed recently. The advantage of the MC method is that no information on the derivatives is required. This is very convenient when other observables (e.g., $B(E2)$ values) are included in the fitting. As a comparison, the singular value decomposition (SVD) approach is also employed in the fitting process. We have 20 variables in total. The fitting was carried out in three steps. In the first step we only consider 131 states in the nuclei $^{102-112}$Sn and $^{120-132}$Sn. The nuclei $^{113-114}$Sn and $^{118-119}$Sn are considered in the second step to further fine-tune the effective interaction. The three isotopes $^{115-117}$Sn are added to the calculation in the last step [1]. Diagonalizations are done within the so-called $M$-scheme with a parallel shell model program we developed a few years ago [15].

As tests, calculations are done with 10 sets of random monopole Hamiltonians. They are generated by the Monte Carlo sampling approach and are optimized by fitting to the 131 states mentioned above. We found that in all cases one can get convergence with the MC approach within ten iterations, as seen in the left panel of Fig. 1 where one set of these calculations is presented. In the right panel of Fig. 1 the same calculations are done starting from the realistic CD-Bonn potential.

![Figure 1](image.png)

**Figure 1.** Left: Convergence of the mean-square deviations $\chi^2$ within the SVD and MC approaches for calculations with a random monopole Hamiltonian; Right: Same as the left but for calculations with the CD-Bonn potential [1].

The monopole Hamiltonians we derived in Fig. 1 are slightly refined by including into the fitting the nuclei $^{113-119}$Sn. We include a total number of 157 states in the fitting [16, 17]. After around 15 iterations both calculations give a mean-square deviation $\chi^2 \sim 2.35$ MeV. It means that these states can be reproduced within an average deviation of about 123 keV. The monopole Hamiltonians optimized with the SVD and MC approaches are similar to each other. The largest uncertainties of the optimized monopole Hamiltonian are related to the single-particle energies. The values predicted by the MC approach are $\varepsilon_{1d_{5/2}} = 5.013 \pm 3.10$, $\varepsilon_{2s_{1/2}} = 0.369 \pm 2.63$ and $\varepsilon_{0h_{11/2}} = 3.249 \pm 0.83$ MeV.

In Fig. 2 we plotted the deviation from experimental data for calculations with the two effective Hamiltonians. The difference between the calculations is practically negligible. The largest deviation from experiments, denoted as $r$ in Fig. 1, is seen at $N = 15$ where the ground
The calculated shell model energies, $E_{SM} = \langle H \rangle$, of the selected states in tin isotopes are plotted in the right panel of Fig. 2. The contributions from the monopole Hamiltonian are also presented for comparison. The comparison between experimental and calculated binding energies of the ground states in Sn isotopes is plotted in Fig. 3.

The excitation energies of the 126 excited states can be reproduced within an average deviation of about 150 keV. The largest difference is seen in the $3/2^+$ state in $^{115}$Sn mentioned above, where the experimental datum is under-estimated by about 540 keV. Extensive experimental efforts are made recently to explore higher-seniority states built on the $10^+$ states in Sn isotopes. The calculated excitation energies of the $11/2^-, 1/2^+, 5/2^+$ and $7/2^+$ one-neutron-hole states in $^{131}$Sn, relative to the $3/2^+$ state, are -0.022, 0.475, 1.720 and 2.521 MeV, respectively.

Detailed systematic calculations on the spectra and decay properties of tin isotopes as well as the list of the two-body matrix elements will be presented in Ref. [18]. We have done a preliminary optimization of the $T = 0$ monopole interaction by fitting to the binding energies of Sb, Te and I isotopes around the $N = 50$ and 82 shell closures. This will also be available in Ref. [18].

The spins of the ground state and first excited state in $^{103}$Sn are $I = 5/2$ and $7/2$, respectively, which are reversed with respect to those in $^{101}$Sn [14]. Ref. [14] suggested that the inversion is dominated by orbital-dependent pairing correlations, namely the strength of the pairing matrix.
elements $\langle 0g_{7/2}^2 | V | 0g_{7/2}^2 \rangle_{J=0}$ is much larger than that of $\langle 1d_{5/2}^2 | V | 1d_{5/2}^2 \rangle_{J=0}$. This produces strong additional binding for the $J^\pi = 5/2^+$ state in $^{103}$Sn, which eventually becomes the ground state. The effect of other interaction terms on the spin inversion was not considered in Ref. [14]. In Fig. 4 we analyze the contribution from different components of the effective Hamiltonian to the spin inversion between $^{103}$Sn and $^{103}$Sn. For that purpose the energies of the first $J^\pi = 5/2^+$ and $7/2^+$ states are calculated with a limited Hamiltonian $H'$ containing the single-particle terms and two-body matrix elements with $J \leq J_{\text{max}}$ only, where $J_{\text{max}}$ denotes the maximal spin value of the two-body matrix elements to be considered. Two different types of calculations are presented in the figure. The solid symbols correspond to the results calculated by diagonalizing the Hamiltonian $H'$. The expectation values of such a Hamiltonian with respect to the corresponding wave functions $|\Psi_I\rangle$ of the full Hamiltonian $H$, $\langle \Psi_I | H' | \Psi_I \rangle$, are plotted as open symbols. It is thus seen from Fig. 4 that both calculations give similar results concerning the order of the $5/2^+$ and $7/2^+$ states. Calculations with the pairing matrix elements only (i.e., $J_{\text{max}} = 0$) show that the pairing terms, in particular the element $\langle 0g_{7/2}^2 | V | 0g_{7/2}^2 \rangle_{J=0}$, mentioned above, can significantly reduce the gap between the two states but were not strong enough to induce the inversion. A sudden switch is seen when the $J = 6$ two-body matrix elements are considered.

It can be seen from Fig. 4 that in both calculations the exact results are also approached by including terms with $J \leq 6$ only. This is expected since the low-lying states of light tin isotopes mainly occupy the nearly degenerate orbitals $0g_{7/2}$ and $1d_{5/2}$ for which the maximal spin is $J = 6$. Among the $J = 6$ two-body matrix elements the ones that contribute most to the spin inversion are the repulsive matrix element $\langle 0g_{7/2}^2 | V | 0g_{7/2}^2 \rangle_{J=6}$ and the strongly attractive one $\langle 0g_{7/2}^2 1d_{5/2} | V | 0g_{7/2}^2 1d_{5/2} \rangle_{J=6}$. This can be understood by considering the structure of the wave functions of the two states. In the $5/2^+$ ground state in $^{103}$Sn, the leading component is $\langle (0g_{7/2}^2)_{J=0} 1d_{5/2} \rangle I$ [14]. Its overlap with the total wave function is calculated to be $\langle (0g_{7/2}^2)_{J=0} 1d_{5/2} | \Psi_I \rangle I = 0.86$. One can also construct a three-body state starting from the pair $\langle 0g_{7/2}^2 1d_{5/2} \rangle_{J=6}$. The overlap between the state thus constructed and the total wave function is $\langle (0g_{7/2}^2 1d_{5/2})_{J=6} 0g_{7/2}^2 | \Psi_I \rangle I = 0.75$. The $\langle 0g_{7/2}^2 1d_{5/2} | V | 0g_{7/2}^2 1d_{5/2} \rangle_{J=6}$ term induces a significant additional binding for the $J^\pi = 5/2^+$ state in $^{103}$Sn, as is illustrated in the right panel of Fig. 4. It should be mentioned that states generated by the two couplings $\langle (0g_{7/2}^2)_{J=0} 1d_{5/2} \rangle$ and $\langle 0g_{7/2}^2 1d_{5/2} \rangle_{J=6} 0g_{7/2}^2 \rangle I$ are not perpendicular to each other. Their overlap is quite large, $\langle (0g_{7/2}^2)_{J=0} 1d_{5/2} | (0g_{7/2}^2 1d_{5/2})_{J=6} 0g_{7/2}^2 \rangle I = 0.74$. This can be evaluated analytically [19, 20, 21, 22].

**Figure 4.** Left: The calculated shell-model energies of the first $5/2^+$ and $7/2^+$ states in $^{103}$Sn with a Hamiltonian $H'$ containing the single-particle terms and two-body matrix elements with $J \leq J_{\text{max}}$; Right: A schematic plot on the effect of configurations with high $J$ values.
The overlaps of the total wave function of the first $7/2^+$ state $^{103}\text{Sn}$ with its leading components are calculated to be $|(1d_{5/2})_{J=0}0g_{7/2}|\Psi\rangle| = 0.65$, $|(0g_{7/2}2)J=0g_{7/2}|\Psi\rangle| = 0.62$ and $|(0g_{7/2}1d_{5/2})J=61d_{5/2}|\Psi\rangle|=0.57$. From a shell-model point of view, the couplings $|(0g_{7/2})_{J=0}0g_{7/2}|_I$ and $|(0g_{7/2})_{J=6}0g_{7/2}|_I$ generate exactly the same three-particle state. All interaction terms $\langle0g_{7/2}V|0g_{7/2}\rangle_J$ contribute to the total energy of the state [19]. It may be interesting to mention that the effect of the maximally aligned pair in single-$j$ systems was discussed in Refs. [19, 23, 24].

In summary, the structure properties of light tin isotopes are calculated with a global optimized effective interaction. The unknown single-particle energies of the orbitals $1d_{3/2}$, $2s_{1/2}$ and $0h_{11/2}$ and the monopole interactions are refined by fitting to experimental binding energies. A total number of 157 states in $^{102-132}\text{Sn}$ are considered in the fitting. The binding energies of these states can be reproduced within an average deviation of about 120 keV. The largest deviation is around 400 keV which is seen in the nucleus $^{115}\text{Sn}$. With the effective Hamiltonian thus derived we analyze the origin of the spin inversion between the $7/2^+$ and $5/2^+$ states in $^{103}\text{Sn}$ and heavier odd tin isotopes in order to explore the possible influence of different interaction channels. We thus find that both the $J = 0$ pairing and the maximally aligned $J = 6$ two-body matrix elements produce strong additional binding for the $5/2^+$ states. The non-diagonal pairing matrix elements play an essential role in inducing the mixing of different configurations in the wave functions of these states.

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