Effect of $0h_{11/2}$ Level on Shell Model Calculations of ^{105}Sb and ^{107}Sb

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The full and reduced shell model calculations have been carried out for the light odd–even ^{105}Sb and ^{107}Sb isotopes. The model space has been chosen as $1d_{5/2}$, $0g_{7/2}$, $1d_{3/2}$, $2s_{1/2}$, and $0h_{11/2}$ for the full calculations and excluded $0h_{11/2}$ for the reduced calculations. The reduced shell model calculations of ^{105}Sb and ^{107}Sb isotopes are presented for the first time. We obtain the energy spectra for the ^{105}Sb and ^{107}Sb isotopes in the full and reduced model space by using CD-Bonn two-body effective nucleon–nucleon interaction. The resulting energy spectra are compared to the experimental results to understand the effect of the $0h_{11/2}$ level on the shell model calculations. We draw conclusions about the right model space in the shell model calculations for the isotopes around the $N = Z = 50$ region of the periodic table.

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The nuclear structure physics community has devoted much experimental and theoretical efforts to explore the structure of the nuclei close to the limit of stability over the last many years. The odd–even nucleus ^{105}Sb was found experimentally to be the lightest ground state emitter a few years ago.[1] Experimental studies of the next available odd–even nuclei ^{107}Sb and ^{109}Sb have been performed just a few years ago before the investigation of ^{105}Sb.[2–5] The full shell model description of low-lying states for these nuclei has been proposed for ^{105}Sb, ^{107}Sb in Refs. [6, 7], and for ^{109}Sb in Ref. [8]. The full shell model description of these nuclei contains up to 9 valence nucleons in the *sdgh* major shell which has the single particle states $2s_{1/2}$, $1d_{5/2}$, $1d_{3/2}$, $0g_{7/2}$, and $0h_{11/2}$. The next odd–even nucleus ^{111}Sb which contains 11 valence nucleons in the *sdgh* major shell has not been able to be studied yet because of numerical difficulties. Addition of the single particle orbit $0h_{11/2}$ and even one more nucleon to the model space enormously increase the calculations of the coefficient of fractional parentage (CFP) and the dimensions of the Hamiltonian matrices. The J value of the $0h_{11/2}$ orbit is the largest one within the model space. Thus, the major contribution to the CFP calculations and the Hamiltonian calculations comes from this orbit. This makes sometimes the shell model calculations impossible, since today's computer technology is not enough for a single computer to do that kind of huge numerical calculations. The question being considered in this point of view is how we can predict the ground states and some excited states of the heavier isotopes such as ^{110}Sb, ^{111}Sb, ^{109}Sn, ^{110}Sn, etc. in the $N = Z = 50$ region. If we reduce the model space, this enables us to do the shell model calculations for those kinds of nuclei. For this purpose, we need to check whether the reduced shell model calculations are capable of reproducing the experimental results for the nuclei whose shell model calculations can be carried out in the full model space. The only possible targets for the Sb isotopes, having experimental data, in the $N = Z = 50$ region are the ^{105}Sb and ^{107}Sb isotopes. If we obtain good results at low-lying energy levels compared to experimental results, we can use this reduced model space to predict the ground state and a few excited states of the nuclei which have more than 9 valence nucleons, within the framework of shell model.

This work aims to see whether shell model calculations, based on two different model spaces, i.e. *sdgh* and *sdg*, are capable of reproducing the experimental results for the nuclei close to the stability line. The shell model calculations for the odd–even nuclei ^{105}Sb, ^{107}Sb, ^{109}Sb have been performed by using the full model space so far. The next nuclei ^{110}Sb, ^{111}Sb which contain 10 and 11 nucleons in the *sdgh* major shell have not been amenable to study, since no computer code is able to construct their Hamiltonian matrices in the full *sdgh* model space basis so far. The main reason is the huge dimensions of the Hamiltonian matrices. In this Letter, we use, for the first time to my knowledge, the reduced model space which significantly reduces the dimensions of the Hamiltonian matrices, in order to see whether shell model calculations based on this model space are capable of reproducing the experimental results for the nuclei ^{105}Sb and ^{107}Sb. It is also important to check the validity of the shell model calculations in different model spaces in the $A = 100$ region. If the reduced model space gives the reasonable results in this region of the periodic table, we can extent the studies to predict the ground state and a few excited states for heavier nuclei in this region, i.e. ^{111}Sb, using smaller model spaces. Before we present our results, we briefly review how to perform the shell model calculations.

The shell model problem aims at solving the many-body system in a set of valence shells in terms of in-

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dependent particle wave functions with the dynamics specified by the Hamiltonian

$$H = \sum \epsilon_\alpha a^\dagger_\alpha a_\alpha + \sum V^{effective}_{\alpha\beta\gamma\delta} a^\dagger_\alpha a^\dagger_\beta a_\gamma a_\delta. \qquad (1)$$

The solution implies deriving systematically the energy spectra, electromagnetic transitions, and beta decay of series of nuclei in specific region of the periodic table.

The Drexel University Shell Model (DUSM) code was introduced almost 15 years ago[9] as a different approach to perform multi-shell nuclear shell model calculations. It addresses the solution of the Hamiltonian 1 for a specific nucleus, giving an effective interaction. It is based on a separation of the various subspaces in which the single particle wave functions are defined. This is achieved via extensive use of permutation group concepts and a redefinition of the CFP to include permutation labels. This leads to a modern efficient approach to the nuclear shell model.

This algorithm is based on extensive use of permutation group concepts. In this method the Hilbert space is separated into two parts: the orbital angular momentum (J) and isospin (T). A state with good isospin belongs to arbitrary irreducible representations (irrep) of the symmetric group and appropriate orbital angular momentum states belong to the conjugate irrep. The restriction of the isospin irreps to two rows ($t = 1/2$) implies a restriction of the orbital angular momentum irreps to two columns. By using the inner-product isoscalar factor we form globally antisymmetric states from states that belong to two conjugate irreps. This procedure enables us to efficiently construct a full $J - T$ basis.

The CFPs are calculated separately for N particles in spin (J) and isospin (T) spaces. The N-particle states obtained from symmetric or antisymmetric $(N-1)$-particle states by coupling of one more particle can belong to any permutational symmetry. The procedure involves the construction and diagonalization of the matrices representing the quadratic Casimir operators for the appropriate unitary and orthogonal groups. The CFPs of the antisymmetric $J - T$ coupled states are obtained in terms of products of the CFPs for J and T corresponding to conjugate representations of the symmetric group. Consequently, the common eigenvectors of the quadratic Casimir operators in this approach are the CFPs, and the eigenvalues specify the permutational symmetry and the seniority.[10] Redefinition of the CFPs by introducing the new permutational group labels and the angular momentum labels saves a lot of the computation in this procedure because the dimensions of the involved matrices are never very large, since the dimensions of the permutation group representations are not so large. Thus this gives less number of the coupled angular momenta values and presumably great saving of the computation time.

In the following stage, the coupling coefficients and the isoscalar factors for the inner and outer products of wave functions of arbitrary symmetry in the different subspaces are recursively calculated to form a global antisymmetric multi-particle multi-shell wave function. Finally the Hamiltonian matrix is calculated by using the elementary matrix elements, the coupling coefficients for the inner and outer products, the given single particle energies, and potential matrix elements in the basis.

In order to obtain the eigenvalues of the Hamiltonian matrix, the DUSM code uses the Lanczos diagonalization procedure,[11] an iterative method which gives the solution of the lowest eigenstates. The Lanczos method is included in the construction of an orthogonal basis in which the Hamiltonian matrix is tridiagonal. The real symmetric matrix is diagonalized at each iteration and the iterative process continues until all the required eigenvalues are converged.

The shell model calculations have been performed with two possible model spaces. In the harmonic oscillator configuration with the spin-orbit coupling, $0h_{11/2}$ level comes down from $5\hbar w$ energy quanta. Therefore, in the $N = Z = 50$ region, the $sdgh$ major shell includes the single particle state $0h_{11/2}$. The model space in the shell model calculations can be assumed to be either the one which comprises all single particle states of the $2s_{1/2}$ $1d_{3/2}$ $1d_{5/2}$ $0g_{7/2}$ $0h_{11/2}$ shell or the one which excludes the $0h_{11/2}$ state.

This work aims to decide which model space, i.e. $sdgh$ or sdg, gives better agreement with the experimental results. This decision may help us to do shell model calculations for heavier isotopes near $A = 100$ region. Because the exclusion of the $0h_{11/2}$ level from the model space reduces significantly the amount of calculations. The latter model space was also used in the shell model calculations in Ref. [12]. Since there is no experimental information available for the nuclei one particle away from the closed shell nucleus ^{100}Sn to extract the single particle energies, we choose the single particle energies as $\epsilon_{2s_{1/2}} = 2.45$ MeV, $\epsilon_{1d_{3/2}} = 2.55$ MeV, $\epsilon_{1d_{5/2}} = 0.00$ MeV, $\epsilon_{0g_{7/2}} = 0.08$ MeV and $\epsilon_{0h_{11/2}} = 3.20$ MeV. These energies give reasonable results for the light and medium heavy Sn nuclei in the $A = 100$ region.[6] We have used the effective two-body interactions CD-Bonn, provided by Hjorth–Jensen in private communication, to calculate low-lying energy levels.

Table 1 gives explicitly the available experimental values and the theoretical ones up to 3 MeV. There are also more theoretical states than those reported in the enclosed table. Here all states up to 1 MeV and after 1 MeV only the ones corresponding to experimental levels are reported. We plot the low-lying energy levels in Fig. 1 for ^{105}Sb, in Fig. 2 for ^{107}Sb, for the two different model spaces together with the experimental levels reported in Ref. [1,2]. The full model space

includes all single particle states $2s_{1/2}$, $1d_{3/2}$, $1d_{5/2}$, $0g_{7/2}$, and $0h_{11/2}$. The reduced model space includes the ones excluding $0h_{11/2}$.

Table 1. Experimental and theoretical low-lying states (up to 3.0 MeV) of the odd–even ^{105}Sb and ^{107}Sb isotopes. Theoretical states are obtained by using two model spaces, i.e. full and reduced. Energies are in units of MeV.

^{105}Sb				
J_i^π	Expt.	J_i^π	Full	Reduced
$\frac{5}{2}^+$	0.00	$\frac{5}{2}^+$	0.000	0.000
–	–	$\frac{7}{2}^+$	0.451	0.437
–	–	$\frac{1}{2}^+$	0.462	0.294
–	–	$\frac{3}{2}^+$	0.504	0.317
$\frac{9}{2}^+$	1.22	$\frac{9}{2}^+$	1.172	0.901
$\frac{13}{2}^+$	1.84	$\frac{13}{2}^+$	1.911	1.556
$\frac{15}{2}^+$	2.21	$\frac{15}{2}^+$	2.137	1.844
$\frac{17}{2}^+$	2.50	$\frac{17}{2}^+$	2.429	2.105
$\frac{19}{2}^+$	2.99	$\frac{19}{2}^+$	2.874	2.559
^{107}Sb				
J_i^π	Expt.	J_i^π	Full	Reduced
$\frac{5}{2}^+$	0.000	$\frac{5}{2}^+$	0.000	0.000
–	–	$\frac{1}{2}^+$	0.275	0.099
–	–	$\frac{3}{2}^+$	0.471	0.264
$\frac{7}{2}^+$	0.769	$\frac{7}{2}^+$	0.600	0.552
$\frac{9}{2}^+$	1.058	$\frac{9}{2}^+$	1.035	0.733
$\frac{9}{2}^+$	1.389	$\frac{9}{2}^+$	1.924	1.524
$\frac{11}{2}^+$	1.791	$\frac{11}{2}^+$	1.637	1.274
$\frac{13}{2}^+$	1.900	$\frac{13}{2}^+$	1.865	1.434
$\frac{13}{2}^+$	2.164	$\frac{13}{2}^+$	2.374	1.970
$\frac{15}{2}^+$	2.240	$\frac{15}{2}^+$	2.364	1.957
$\frac{17}{2}^+$	2.536	$\frac{17}{2}^+$	2.667	2.199
$\frac{17}{2}^+$	2.746	$\frac{17}{2}^+$	2.757	2.426

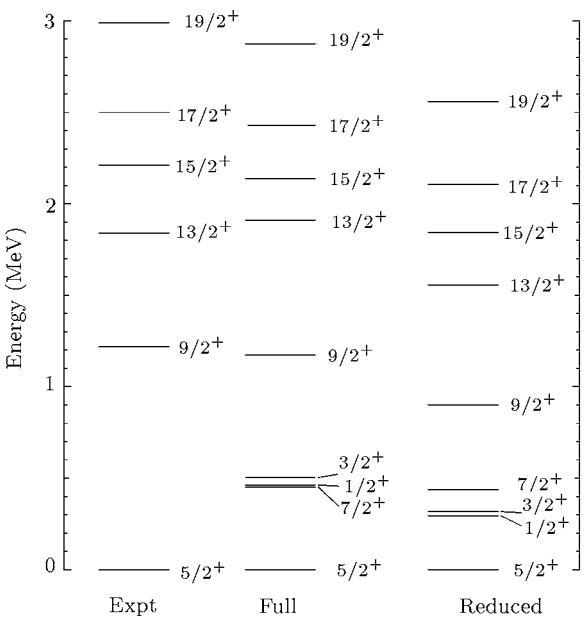


Fig. 1. Experimental and theoretical spectra of ^{105}Sb.

The states obtained by using two different model spaces are almost in the same order. The energy levels obtained from the reduced model space are lower than those of the full model space for both ^{105}Sb and ^{107}Sb. It is expected to be so, since the states obtained from the full model space are a result of the coupling of the $0h_{11/2}$ level which has the highest single particle energy in the full model space. There are three more theoretical extra states below 1 MeV. Unfortunately, these states have not been observed in the experiment. The energies of the state $\frac{7}{2}^+$ for the full and reduced model spaces are so close each other with respect to the other states. That is why $\frac{3}{2}^+$ and $\frac{1}{2}^+$ states go down below the $\frac{7}{2}^+$ state for the reduced model space. The energies of the states $\frac{3}{2}^+$ and $\frac{1}{2}^+$ are lowered down as the same as the other states except the state $\frac{7}{2}^+$. The energy gaps observed experimentally, the ones above the ground state, the $\frac{9}{2}^+$ and $\frac{13}{2}^+$ states, are obtained by the two model spaces. Furthermore, the energy differences between two adjacent levels are larger for the reduced model space than the ones for the full model space.

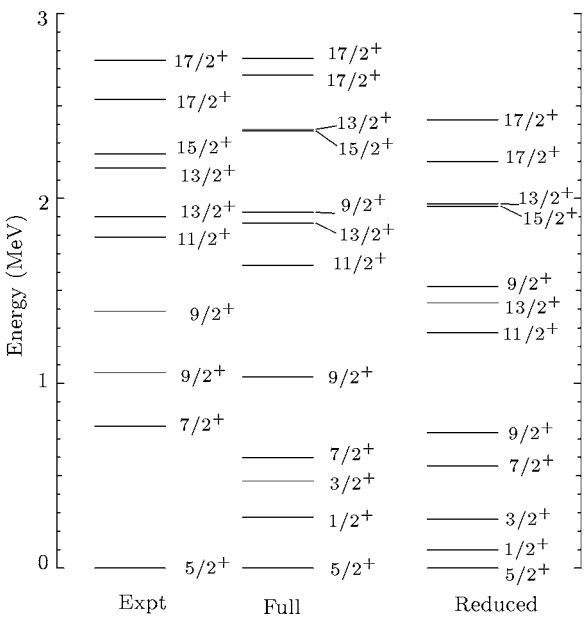


Fig. 2. Experimental and theoretical spectra of ^{107}Sb.

In conclusion, the shell model calculations have been carried out for the odd–even isotopes ^{105}Sb and ^{107}Sb by using two different model spaces to understand the effect of $0h_{11/2}$ states on the calculations. The reduced shell model calculations are presented for the first time here. The full model space including all single particle states, $2s_{1/2}$, $1d_{3/2}$, $1d_{5/2}$, $0g_{7/2}$, and $0h_{11/2}$, gives better agreement with the experimental results than the reduced model space which includes all single particle states excluding $0h_{11/2}$. However, the reduced shell model calculations are reasonable.

The reduced model space gives the levels almost in the same order except the state $\frac{7}{2}^+$ for both ^{105}Sb and ^{107}Sb. This means that the reduced model space can be used to predict the ground state and a few excited states for heavier isotopes, i.e. ^{111,112}Sb, ^{109,110,111}Sn, etc., in the $N = Z = 50$ region. According to our results, the right model space for the shell model calculations in the $N = Z = 50$ region is the full model space. Therefore, there is an effect of the $0h_{11/2}$ level on the shell model calculations of ^{105}Sb and ^{107}Sb. We suggest that the similar calculations are in order for the other isotopes in the $N = Z = 50$ region.

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