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Single-shell states for multi-shell description of nuclei

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Abstract. The DUSM method is described for constructing the single-shell states and the corresponding matrix elements needed for describing the isotopes of a given nucleus within a major shell in the framework of the nuclear shell model. The advantage of this approach is that a streamline set of states are constructed, thereby reducing the calculation requirements. The idea is to truncate the full space of permutational irreducible representations with two columns to subspaces where the second column is restricted in its number of boxes - depending on the isospin value. The usefulness of this method for large-scale shell model calculations in the fp - and $sdgh$ -shell is emphasized. An application to Sn isotopes in the $sdgh$ -shell is presented.

1. Introduction

The nuclear shell model provides systematic descriptions for some series of isotopes within major shells. These studies are particularly important to recognize the systematic trends in the nuclear properties as function of proton or neutron numbers. It became the standard approach for describing the systematics found in the spectra and transition matrix elements of the p -shell nuclei ($1p_{\frac{3}{2}}$ and $1p_{\frac{1}{2}}$) - [1], the sd -shell nuclei ($1d_{\frac{5}{2}}$, $1d_{\frac{3}{2}}$, and $2s_{\frac{1}{2}}$)- [2, 3], the fp -shell nuclei ($0f_{\frac{7}{2}}$, $0f_{\frac{5}{2}}$, $1p_{\frac{3}{2}}$, and $1p_{\frac{1}{2}}$) [4, 5, 6], and the $sdgh$ -shell nuclei ($2s_{\frac{1}{2}}$, $1d_{\frac{5}{2}}$, $1d_{\frac{3}{2}}$, $0g_{\frac{7}{2}}$, and $0h_{\frac{11}{2}}$) [7, 8, 9, 10, 11, 12].

The shell model approach applied to the description of nuclei is notoriously difficult to perform numerically. In particular the study of neutron (proton) rich nuclei demand systematic description of many nucleons systems in large multi-shell spaces. These nuclei are at the focus of the studies performed with the radioactive beam facilities and crucial for astrophysical applications. A major difficulty for the shell model description of these nuclei is the multi-shell basis dimensions which might be enormous. In the m scheme formalism, all the states with angular momentum $J > J_z$ and isospin $T > T_z$ are included in the calculations. This leads to the main difficulty of the m scheme formalism in that the number of basis states becomes very large even for few valence nucleons. The projection onto states of good total angular momentum J and isospin T is achieved automatically due to the Hamiltonian being a scalar. The number of basis states for states of good J and T in the $J - T$ scheme formalism is much smaller than the number of states in the m scheme. The $J - T$ description is clearly advantageous here over the m scheme.

In this contribution, a great simplification in building the model space for the nuclei with large isospin states (stretched or near stretched states) is offered in the Drexel University Shell Model (DUSM) approach developed in $J - T$ scheme [13, 14, 15]. It is based on the limits on the permissible Young partitions describing the states. These limits are exact; yet they are very



difficult to implement in conventional approaches to the shell model. However, it will be shown below a natural framework to implement such a truncation.

2. The DUSM Formalism

A different approach for performing multi-shell nuclear shell model calculations was introduced almost 20 years ago [13, 14, 15]. This algorithm is based on extensive use of permutation group concepts. In this method the orbital angular momentum states and isospin states are treated separately. A state with good isospin belongs to an *arbitrary* irreducible representation (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 ($t = \frac{1}{2}$) implies a restriction of the orbital angular momentum irreps to two columns. By using the inner-product isoscalar factor we obtain globally antisymmetric states from any two states that belong to two conjugate irreps. This procedure enables us to originally and efficiently construct a full $J - T$ basis.

The global orbital states for multi-shell configuration are constructed, by using outer-product isoscalar factors, from single-shell states that also belong to *arbitrary* irreps of the symmetric group. However, since the global orbital states are restricted to two columns irreps, the single shell states are also restricted to these irreps. (In this contribution it is shown that we can put an additional restriction on the number of boxes in the second column, depending on the isospin value.) The one- and two-body matrix elements must then be calculated between states which belong to these conjugate orbital and isospin irreps. The concept of a summation over paths in Young diagram space is used to take into account the contributions from all possible irreps in both orbital and isospin spaces.

The Drexel University Shell Model (DUSM) computer code [15] implemented this new approach to perform shell model calculations in the isospin scheme where the nucleons are distributed in several single-shells. A parallel version of the DUSM code - DUPSM was written [6, 9] using PVM [16], a dynamic environment for parallel programming, supporting the message passing paradigm.

The parallel calculation of the Hamiltonian matrix in the DUPSM code is very efficient since every processor calculates small independent submatrices in which the single-shell states belong to given permutational irreps. In addition, mainly because of the permutational symmetry selection rules, the matrices are sparse (for matrices of order of hundreds of thousands only few percent of the matrix elements are non-zero). With the DUPSM code we can calculate matrices of order of few millions on few tens of parallel machines in a relatively short time.

The DUSM algorithm recursively builds the single-shell many-body states based on the permutation group labels as illustrated in Figure 1. The states are built with a two rows restriction in isospin space and a related two columns restriction in orbital space. The matrix elements of any combination of elementary creation and annihilation operators, from a^+ to a^+a^+a , are then calculated between these states, taking care of all the different paths. These form the building blocks from which to calculate the matrix elements of any one- and two-body operator (Hamiltonian and transition operators) in the multi-shell calculations describing nuclei with *any given value of isospin*.

3. Exact Truncation for Single-Shell Irreps

The DUSM approach offers originally an advantage in Ref. [13, 14, 15] in that the orbital and isospin sub-spaces are separated leading to an enhanced sparsity of the Hamiltonian matrix and to an economy of space for the single-shell one- and two-body operators. This is achieved by restriction of Young frames into two-column irreps including all irreps in Figure 1. Even then extra truncation might be required to render the calculations feasible for the very large Hamiltonian matrix.

An extra exact truncation is presented in this contribution: the restriction of the Young frames into the number of boxes in the second-column irreps, e.g., no-box, one-box, two-boxes, etc depending on the isospin value of the nuclei.

Let's start with all the isotopes with T_{max} i.e., stretched (maximum) isospin. For example, the Ca isotopes in the fp -shell and the Sn isotopes in the $sdgh$ -shell. For any given number n of valence nucleons (actually, only neutrons - no valence protons in these cases) the appropriate isospin state belongs to the permutational irrep $[n]$, i.e., one row with n boxes. Therefore, its adjoint states should belong to the permutational irrep $[111...11]$, i.e., one column irreps with n boxes - below the blue line in Figure 1. Consequently, all the single-shell irreps must also have only one column. It is trivial to justify that we can take just these one column irreps since by removing one box from any given one column irrep we can get only another one column irrep with one less box - see Figure 1. This truncation is *exact*.

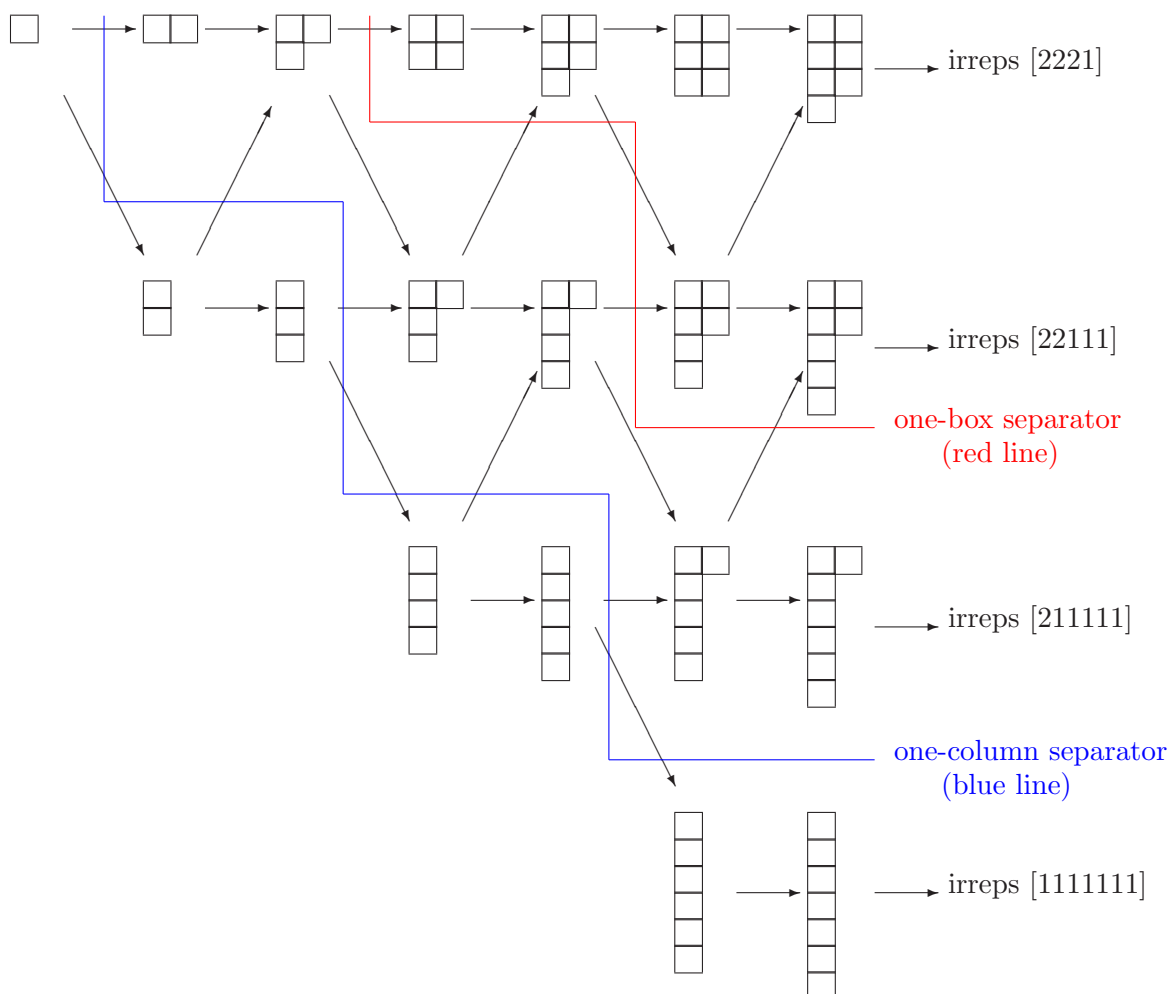


Figure 1. Two columns irreps for 1-7 particles. The arrows indicate irreps connected by the addition of one-box. The red line splits between the irreps with at most one-box in the second column and those with more than one-box. The blue line splits between the irreps with one-column and those with more than one-column

Consider *all* the Ca isotopes in the fp -shell; in this case it is sufficient to truncate the $f_{\frac{7}{2}}$ states to those belonging to the irreps $[1]$, $[11]$, $[111]$, \dots $[11111111]$, and the other shells to the $[1]$, $[11]$, $[111]$, \dots , $[111111]$ $f_{\frac{5}{2}}$ states, the $[1]$, $[11]$, $[111]$, and $[1111]$ $p_{\frac{3}{2}}$ states, and the $[1]$ and $[11]$ $p_{\frac{1}{2}}$ states (see irreps below the blue line in Figure 1). The memory required for the single-shell states and the matrix elements related to these irreps is negligible - less than 1MB.

Let's assume that we want to calculate *all* the isotopes with $T_{max} - 1$ in a given major shell, i.e., the Sc isotopes in the fp -shell and the Sb isotopes in the $sdgh$ -shell. In this case the isospin state for a nucleus with n valence nucleons belongs to the irrep $[n - 1, 1]$, i.e., a two-rows irrep with only one-box in the second row. The adjoint irrep is $[211\dots111]$, i.e., a two columns irrep with only one-box in the second column. Therefore, *all* the orbital single-shell irreps should also belong to the irreps with one-box in the second column - see Figure 1. The full space of two-columns irreps is truncated to a subspace which includes only those irreps with at most one-box in the second column, i.e., the irreps between the red and blue lines in Figure 1. This truncation is possible since deleting one-box from any given irrep of the type $[211\dots1111]$ leaves either an irrep of the same type, if we remove the last box from the first column, or a one-column irrep if we remove the box in the second column. Both should be included in the case of $n - 1$ valence nucleons as pointed out in Figure 1.

The Sc isotopes have $T_{max} - 1$ isospin. To calculate an arbitrary nucleus in the middle of the fp -shell would require to include all the single-shell states of $f_{\frac{7}{2}}$ which belong to the 44 two-columns irreps (16 valence nucleons with maximum 8 rows). To model the Sc isotopes it is sufficient to consider only the eight one-column irreps, and, in addition, the eight irreps with two-boxes in the first row i.e., $[2]$, $[21]$, $[211]$, \dots , $[21111111]$ (see irreps between the red and blue lines in Figure 1). For $f_{\frac{5}{2}}$ we have to add only six such irreps, i.e., till $[211111]$, for $p_{\frac{3}{2}}$ we have to add four irreps till $[2111]$, and for $p_{\frac{1}{2}}$ we have to add only the irreps $[2]$ and $[2, 1]$. This truncation is obviously exact.

It is important to note that, actually, for the last case, we are reducing the number of single-shell matrix elements by a factor much larger than $\frac{24}{90}$. The reason is that for more than two particles the number of states included in the one-column irrep is less than those included in the two-columns irrep with one-box in the second column. As the single-particle angular momentum j is becoming larger and more nucleons occupy the shell - much more states are included in the latter irrep. The reason was actually explained above - more irreps contribute to the build-up of the two-columns irreps than the one-column irrep - see Figure 1 (Whereas, only one irrep with one-column contributes to the next one-column irrep, two irreps contribute to the two-columns irrep with one-box in the second column.) Similarly, the number of states in the two-columns irrep with one-box in the second row is less than the number of states included in the irrep with two-boxes in the second row (except for the 4-particle irreps).

A similar truncation can apply to the isotopes with $T_{max} - 2$. In this case we have to add the irreps with two-boxes in the second column to each single-shell. For example, we have to add 7 more irreps to the $f_{\frac{7}{2}}$ single-shell, $[22]$, $[221]$, $[2211]$, \dots , $[22111111]$, for a full multi-shell calculation. Similarly, for the $h_{\frac{11}{2}}$ single-shell we have to add 11 more irreps - starting with $[22]$ and ending with $[221111111111]$. This amounts to keeping only 35 irreps all together and leaving out 55 irreps. This is a major truncation which will enable us to run easily the Te isotopes (as far as the dimension of the Hamiltonian matrix remains manageable.)

This truncation can also be applied to the isotopes with $T_{max} - 3$; this requires adding the permutational irreps with 3 boxes in the second column, and, consequently to add to each sub-shell list of irreps. For example, for the $f_{\frac{5}{2}}$ shell we need to add the irrep $[222]$, which will close the list of all possible irreps for this single-shell. On the other hand, for the $h_{\frac{11}{2}}$ shell we will need to add 10 more irreps - $[222]$ till $[222111111111]$ - and yet still be left with a truncation of

45 irreps - half of all possible irreps.

We can continue with this procedure for $T_{max} - 4$, $T_{max} - 5$, etc., and add in each case an extra box in the second column, until the minimum value of the isospin - T_{min} is reached. It is clear that for this last case we must use all of the two-columns irreps for each sub-shell, with no possible truncation.

4. Application to Sn Isotopes

Sn isotopes in the *sdgh*-shell, including single-particle orbits $2s_{\frac{1}{2}}$, $1d_{\frac{5}{2}}$, $1d_{\frac{3}{2}}$, $0g_{\frac{7}{2}}$, and $0h_{\frac{11}{2}}$, have the stretched isospin with T_{max} . In this case it is sufficient to truncate the $h_{\frac{11}{2}}$ states to those belonging to the 12 one-column irreps [1], [11], [111], ... [111111111111] compared to the 90 two-column irreps. The other shells belong to the $2j + 1$ one-column irreps (where j is the spin of each single-shell); 2 irreps [1], [11] for $s_{\frac{1}{2}}$, 4 irreps [1], [11], [111], [1111] for $d_{\frac{3}{2}}$, 6 irreps [1], [11], [111], ..., [111111] for $d_{\frac{5}{2}}$, 8 irreps [1], [11], [111], ..., [1111111] for $g_{\frac{7}{2}}$.

This great saving of unnecessary calculation of single-shell irreps allows us to calculate the coefficient of fractional parentage (CFP) and to build the many-body basis states for Sn isotopes. The Hamiltonian matrix for a specific J and T of an Sn isotope are then calculated by using the matrix elements of the elementary operators, the coupling coefficients for outer and inner products, and the given single particle and potential matrix elements in the basis. Finally, the Hamiltonian matrix are diagonalized exactly or via the Lanczos algorithm [17] depending on size.

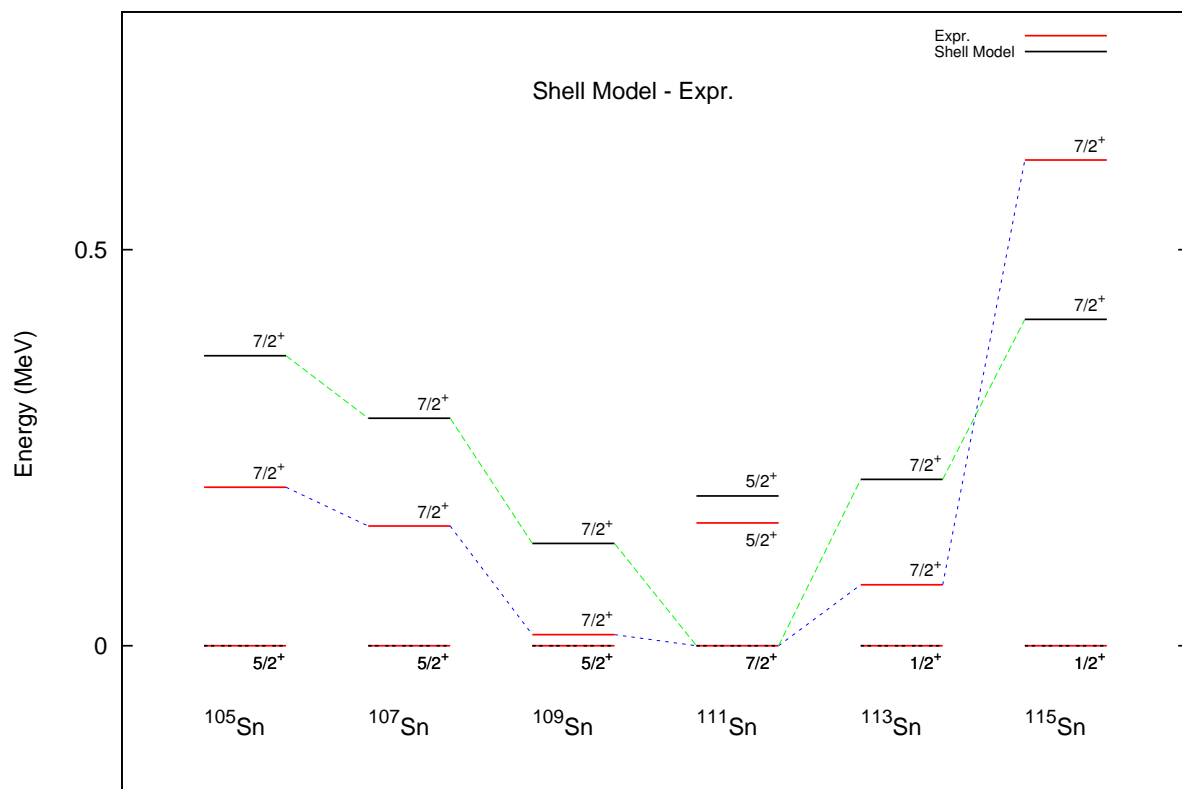


Figure 2. Experimental and theoretical ground state and low-lying state $\frac{7}{2}^+$ of odd-mass Sn isotopes with $A = 105 - 115$.

In our calculations for Sn isotopes we assume that ^{100}Sn is a closed core and let the valence neutrons occupy the single particle orbits $2s_{1/2}$, $1d_{5/2}$, $1d_{3/2}$, $0g_{7/2}$, and $0h_{11/2}$. We have used the CD-Bonn effective interactions as two-body matrix elements given to us by M. Hjorth-Jensen *et al.* [18]. We choose the single particle energies for neutrons as $\varepsilon_{1d_{5/2}} = 0.00$ MeV, $\varepsilon_{0g_{7/2}} = 0.172$ MeV, $\varepsilon_{2s_{1/2}} = 2.45$ MeV, $\varepsilon_{1d_{3/2}} = 2.55$ MeV, and $\varepsilon_{0h_{11/2}} = 3.20$ MeV. The evaluation of the ground states and low-lying state $\frac{7}{2}^+$ of odd-mass Sn isotopes with $A = 105 - 115$ are shown in Figure 2.

5. Conclusion

In conclusion, we presented an algorithm based on the DUSM approach for constructing single-shell states which implements an exact truncation based on the occurrence of only certain Young diagrams in building the multi-shell model states. The rule is that if the isospin is less by n from its maximum value we have to keep the irreps with at most n boxes in their second column. This truncation scheme is extremely important for isotopes with isospin near stretched value. It reduces drastically the necessary number of single-shell one- and two-body matrix elements. This truncation is naturally implemented in the DUSM algorithm to perform shell model calculations since this algorithm is based on the use of the permutation group to build the many-body basis states. This truncation will allow the description of isotopes in the middle of the fp -shell and also of isotopes in the $sdgh$ -shell relatively far from the beginning of the $gdhs$ shell.

The exact truncation described in this contribution are applied to the odd-mass Sn isotopes with $A = 105 - 115$ and found to be very good agreement with experiments. It is a challenging problem to extent these studies to the Sn isotopes with $A = 117 - 120$ including the most stable naturally found ^{120}Sn isotope.

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