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Shell Model Calculations for Even Zirconium Isotopes

S.S. Dimitrova[1], **D. Bianco**[2,3], **N. Lo Iudice**[2,3], **F. Andreozzi**[2,3] and **A. Porrino**[2,3]

[1]Institute of Nuclear Research and Nuclear Energy, Bulgarian Academy of Sciences, 1784 Sofia, Bulgaria

[2]Dipartimento di Scienze Fisiche, Università di Napoli Federico II, Monte S. Angelo, via Cintia, I-80126 Napoli, Italy

[3]Istituto Nazionale di Fisica Nucleare, Sezione di Napoli, Monte S. Angelo, via Cintia, I-80126 Napoli, Italy

Abstract. This contribution is a status report of the project aiming to describe the low-lying structure of the Zr isotopic chain by large scale shell model calculations. An iterative matrix diagonalization algorithm for solving the eigenvalue problem in the m – scheme combined with an importance sampling for an effective truncation of the shell model space is used. The reliability of the method is tested within a large model space spanned by the $(1f_{5/2}, 2p_{1/2}, 2p_{3/2}, 1g_{9/2})$ shells for protons and $(2d_{5/2}, 3s_{1/2}, 2d_{3/2}, 1g_{7/2}, 1g_{9/2}, 1h_{11/2})$ for neutrons. We study the properties of the $N = 96$, 98 zirconium isotopes. In this case a rigorous procedure for truncation the configuration space is required and we implement the importance sampling mentioned above.

1 Introduction

The nuclear shell model is the most adequate tool for describing the low–energy structure of atomic nuclei. The method requires a diagonalization of the Hamiltonian of the system. The sizes of the Hamiltonian matrix increase dramatically as the number of valence shells and/or valence nucleons increases. Thus, a severe truncation of the configuration space is required.

Many truncation methods have been attempted. It may be worth to mention the coupled cluster and the quantum Monte Carlo diagonalization [4] methods. The first was introduced in the 1960s [1] and widely adopted in quantum chemistry (the state-of-art is reviewed in [2]) and nuclear physics (see [3] for the latest results). The second achieves the truncation of the model space by sampling stochastically the basis states.

A newly developed shell model technique [5, 6] was updated recently [7] and applied extensively to study the spectroscopic properties of the $N = 80$ isotones [8] and the heavy Te and Xe isotopes below and above the $N = 82$ shell closure [9–11]. These calculations have shown that the method, dubbed APL, is robust and of easy implementation. The importance sampling the algorithm is

endowed with yields an effective truncation with full control of the accuracy of the solutions.

The long chain of Zr isotopes is a good testing ground for a number of problems like the evolution of the shell structure. There are also new experiments concerning the low lying structure of these nuclei [13,14] which require detailed theoretical studies in this region.

In this contribution, we will discuss a methodological aspect of our project, namely the convergence of the importance sampling for ^{96,98}Zr, where the sizes of the shell model Hamiltonian exceed $N \sim 10^{10}$.

2 The Algorithm

The development of the APL shell model approach went through several steps before being implemented to large–scale shell model problems. The first one was the introduction of an iterative method for generating a subset of eigenvectors of large matrices as an alternative to the Lanczos and Davidson algorithms. We will outline just the key elements of the procedure. A more complete and detailed description can be found in [5].

Let us consider the simplest possible case of a symmetric matrix representing a self-adjoint operator $\hat{A}$ in an orthonormal basis $\{\mid 1\rangle, \mid 2\rangle, \ldots, \mid N\rangle\}$. We will look for the lowest m eigenvectors of the matrix. There are two major stages of the algorithm: an initialization loop and a subsequent set of refinement loops. The initialization begins with diagonalizing the matrix (a_{ij}) (i,j = 1, n), whose sizes n fulfill the relation $(m < n \ll N)$. The lowest m eigenvalues λ_i and eigenvectors $\mid \phi_i\rangle$, are used for constructing the next matrix to be diagonalized

$$\alpha = \begin{pmatrix} \lambda & b_j \\ b_j & a' \end{pmatrix}. \tag{1}$$

This takes into account the next portion of configuration states from $(n+1)$ to n'. In Eq. (1) $\{\lambda\}$ is a diagonal block containing the eigenvalues $(\lambda_i^n, i = 1, m)$, $\{b_j\}$ is a block with elements $b_{ij} = \langle\, \phi_i^n \mid \hat{A} \mid j \,\rangle$ where $(i = 1, m; j = n+1, n')$, and the matrix element of a' are $a'_{jj'} = \langle j \mid \hat{A} \mid j' \rangle$ with $(j, j' = n+1, n')$. Its lowest eigenvalues $\lambda_i^{n'}$ together with the corresponding eigenvectors $\mid \phi_i^{n'}\rangle$ are further used to build a matrix, analogous to α (1), for the next subset of the orthonormal states $\mid j\rangle$. This initialization loop ends when the whole configuration space is exhausted. As a result a zero order approximation for the lowest eigenvalues and eigenvectors is obtained

$$E_i^{(0)} \equiv \lambda_i^N, \quad \mid \psi_i^{(0)}\rangle \equiv \mid \phi_i^N\rangle = \sum_{j=1}^{N} c_j^{(N)} \mid j\rangle \;, \quad \{i = 1, m\}. \tag{2}$$

They are used as an entry to the first refinement loop, which goes through the same steps as describes above. One should just solve an eigenvalue problem of

general form, since the vectors $\mid \phi\rangle$ and $\mid j\rangle$ are no longer orthogonal. It has been shown in [5] that the eigenvalues $E^{(n)}$ and eigenvectors $\mid \psi^{(n)}\rangle$ obtained after the n-th loop converge to the solution of the exact diagonalization of $\hat{A}$.

The second important step towards the implementation of APL method to large-scale shell model problems is the choice of a sampling criterion for reducing the sizes of the configuration space. Bearing in mind that the algorithm provides quite accurate solutions already after the initialization loop, one can sample the configuration space as follows:

- Diagonalize the submatrix $\{a_{ij}\}$ $(i,j=1,m)$ and obtain its eigenvalues λ_i;
- For $j = m+1, \ldots, N$, diagonalize the $m+1$-dimensional matrix

$$\alpha = \begin{pmatrix} \Lambda_m & \vec{b}_j \\ \vec{b}_j^T & a_{jj} \end{pmatrix}, \tag{3}$$

  where $\vec{b}_j = \{b_{1j}, b_{2j}, \ldots, b_{mj}\}$.

- Accept the new state only if

$$\sum_{i=1,m} \mid \lambda_i' - \lambda_i \mid > \epsilon \,, \tag{4}$$

  otherwise ignore the state and continue the sampling process with a new vector j. In the above relation, ϵ is a small parameter which allows to control the accuracy of the truncation. In the actual calculations we use an upgraded important sampling procedure [12].

As it is seen, the two key elements of APL – the approximate diagonalization of large matrices and the importance sampling are closely related. The algorithm provides robust and always ghost–free solutions and the accuracy of the truncation procedure is fully under control. A number of tests for various shell model problems discussed in [6] supports this statement.

3 Convergence of the Method

The aim of the APL approach is to solve shell model problems in large configuration space where the diagonalization even for just few eigenvectors is beyond the capacity of the recent computational facilities.

We perform shell model calculations in the m-scheme within the full model space $(1f_{5/2}, 2p_{1/2}, 2p_{3/2}, 1g_{9/2})$ for protons and $(2d_{5/2}, 3s_{1/2}, 2d_{3/2}, 1g_{7/2}, 1h_{11/2})$ for neutrons. This means that we consider the Zr isotopes as composed of 12 valence protons and n valence neutrons external to the $Z = 28$ and $N = 50$ cores, respectively. The shell model eigenvalue problem can be solved exactly only for the lightest Zr isotopes. It is obvious that for ^{96}Zr and beyond, a severe

truncation of the configuration space is required. In [17] for example, although the space is the same considered here, it is imposed that four particles at most can be allocated in the $1h_{11/2}$ subshell and only states of seniority 8 at most are considered.

Here we perform for first time large scale calculations in the full configuration space mentioned above. The dimensions of the model space for several states of ^{96}Zr and the ground state of ^{98}Zr are listed in Table 1. In order to reduce the sizes of the Hamiltonian matrix we adopt the importance sampling and study the convergence of the iterative procedure to the lowest energy eigenvalues.

Table 1. Dimensions of the shell model space in the m-scheme for several states of ^{96}Zr and the ground state of ^{98}Zr.

Nucleus	J^π	dimension
^{96}Zr	0^+	14 872 779 180
^{96}Zr	2^+	14 411 129 798
^{96}Zr	4^+	13 107 616 806
^{98}Zr	0^+	162 778 727 590

We adopt as two-body potential a renormalized $G-$matrix deduced from the "CD-Bonn" nucleon-nucleon interaction. This realistic effective potential is produced by the code of M. Hjorth-Jensen [15]. Moreover, we use a unique set of single particle energies, the one listed in Table 2.

Table 2. Single particle energies in MeV.

Protons		Neutrons	
$1f_{5/2}$	-10.0	$2d_{5/2}$	0.0
$2p_{3/2}$	-10.5	$2d_{3/2}$	1.0
$2p_{1/2}$	-8.2	$1g_{7/2}$	2.3
$1g_{9/2}$	-7.6	$3s_{1/2}$	2.5
		$1h_{11/2}$	3.5

In order to render the numerical procedure more efficient we perform an effective projection of the total angular momentum by using the modified Hamiltonian

$$\tilde{H} = H - \alpha \left[\hat{\mathbf{J}}^2 - J(J+1) \right]^2 ,$$

where $\hat{J}$ is the total spin operator and α is a positive constant. For a sufficiently large α, this additional term pushes at high energy the states with total spin different from J. Thus, the low-lying spectrum is composed exclusively of levels of spin J.

In Figure 1 we present the behavior of the energy (left panel) and the total spin $\langle J \rangle$ (right panel) for the lowest $J^\pi = 0^+$ states in ^{96}Zr as a function of the

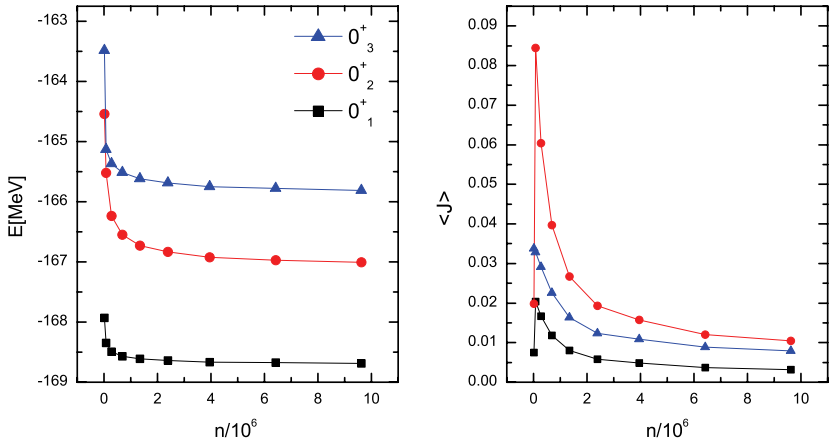

Figure 1. Convergence of the energy (left panel) and spin $\langle J \rangle$ (right panel) for the lowest $J^\pi = 0^+$ states in ^{96}Zr as a function of the size of the Hamiltonian. This is determined uniquely by the sampling parameter ϵ in Eq. 4.

sizes of the Hamiltonian matrix. It is seen that one can reach a saturation of the energy and of the total spin by selecting just $\sim 10^6$ of the totality of basis states. The figures show also that the energies converge faster than the spin. The reason resides in the fact that the basis states probed by the spin are fewer and sparse over the full space.

Figure 2 shows that the convergence rate is also very fast for the energies of the low lying $J^\pi = 2^+$ and 4^+ states in ^{96}Zr.

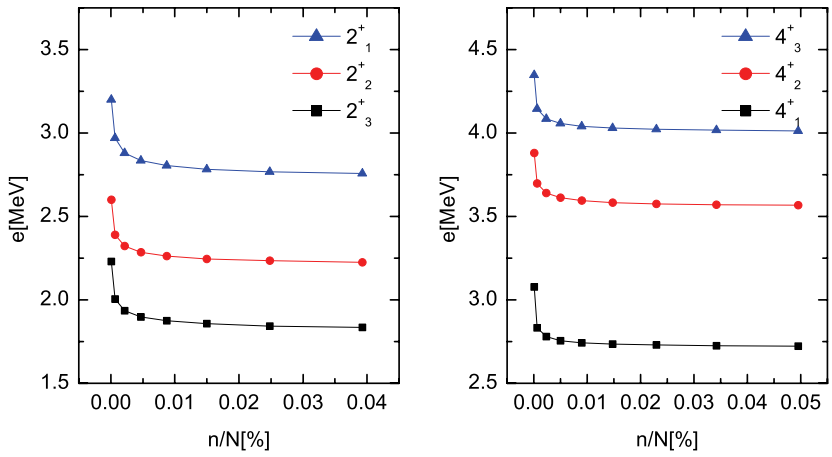

Figure 2. Convergence rate of the lowest $J^\pi = 2^+$ and 4^+ energy levels in ^{96}Zr. The n/N variable is the ratio between the dimensions of the sampled over the full space

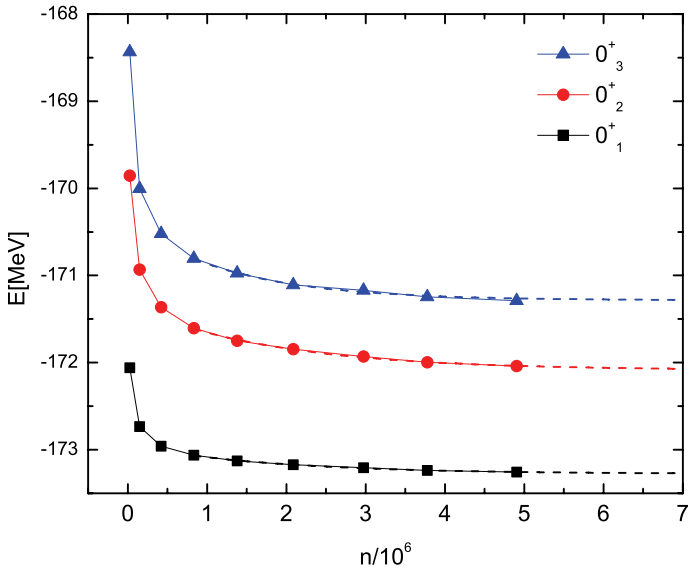

Figure 3. Convergence of the energy of the lowest $J^\pi = 0^+$ states in ^{98}Zr.

Finally, we face the shell model problem in ^{98}Zr. For this isotope, the model space has the prohibitive dimensions $N \sim 10^{11}$. Figure 3 shows that the dimensions of the sampled Hamiltonian matrix is only of the order $n \sim 10^6$. It may be worth to point out once again that the sampling explores the full configuration space.

The good convergence properties obtained for all Zr isotopes, especially for the heavier and most challenging ^{98}Zr, prove that the APL method is extremely efficient and can be safely applied to medium and heavy nuclei.

Moreover, the smooth behavior of the energy curves may allow extrapolation to the asymptotic values. Figure 3, indeed, shows that the sampled data are fitted very well by the function

$$E(n) = E_0 - A\exp(-n/t). \tag{5}$$

Table 3 offers a more detailed comparison. The extrapolated values of the first three $J^\pi = 0^+$eigenvalues E and excitation energies e agree very well with the energies obtained by the extrapolation function.

This function is different from the exponential extrapolation law proposed in [6]. On the other hand, it might well be that the extrapolation laws depend on the specific problem under exam.

Table 3. Calculated and extrapolated values of the lowest eigenvalues of the Hamiltonian E and the excitation energies e for the $J^\pi = 0^+$ states in ^{98}Zr.

Nucleus	E	E_0	e	e_0
0_1^+	-173.256	-173.277	0.000	0.000
0_2^+	-172.039	-172.087	1.217	1.190
0_3^+	-171.288	-171.284	1.968	1.993

4 Conclusions

The results reported here show that the iterative APL method for diagonalizing large matrices is of easy implementation and, combined with the inherent important sampling, offers an efficient tool for solving the shell model eigenvalue problem in very large spaces.

This statement finds confirm in the illustrative examples, presented here, concerning ^{96,98}Zr. We have shown that convergence to the eigenvalues of the Hamiltonian can be reached by just a fraction of the total configurations. Moreover, the curves leading asymptotically to the energy eigenvalues can be fitted by a simple exponential law. This suggests that the method may allow to extrapolate the curves resulting from the iterative procedure to the exact solutions even when the model space is too large to be fully and thoroughly covered by the sampling.

We can therefore state confidently that the implementation of the proposed method can widen the area of application of the shell model to nuclei with large number of valence nucleons in very large configuration spaces.

The future effort within this project will be focused on the systematic study of the spectroscopic properties of the Zr isotopes.

Acknowledgements

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