NUCLEAR THEORY, Vol. 30 (2011)
eds. A. Georgieva, N. Minkov, Heron Press, Sofia

Shell-Model Calculations for ^{91}Zr

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Abstract. The Zr isotopes are often used as a test ground for theoretical studies. Their observed properties change smoothly in going from the spherical ^{90}Zr to the strongly deformed ^{102}Zr. A good description of the low lying excited states in this region can be achieved by performing shell model calculations using interactions based on realistic NN forces. We will report preliminary results on the spectrum of ^{91}Zr within the Important sampling approximation in 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.

1 Motivation

An iterative diagonalization algorithm was proposed recently as a new tool for performing large scale shell model calculations [1,2]. The method, dubbed APL, is robust and of easy implementation. It is also endowed with an importance sampling which yields an effective truncation of the shell model space while the accuracy of the solutions is under full control.

Several tests for various shell model problems, discussed in [2], illustrate the characteristics of the method. The first results of the application of the APL to shell model problems in the $m-$scheme were reported in [3, 4]. The nucleus ^{48}Ca is considered as a system of eight valence nucleons, four protons and four neutrons, above the ^{40}Ca core. The values of the excitation energies and some transition probabilities as a function of the sampling parameter converge fast to the exact eigensolutions obtained by the diagonalization of the full Hamiltonian matrix. These results encouraged us to apply the APL to larger shell model spaces, which are accessible only by cutting severely the shell model basis.

The long chain of Zr isotopes spans from the lightest closed shell nucleus ^{90}Zr to the heaviest so far ^{102}Zr at the neutron drip line. Their low–lying spectra have been object of intensive experimental studies [5] which raised a series of questions, like the evolution of the shell structure and the nature of the mixed symmetry states. These questions need to be faced from a theoretical point of view. The APL algorithm may provide an efficient tool for studying the spectroscopic properties of the first few isotopes of the chain. Here we report on the first preliminary results of a calculation based on this algorithm.

2 The Shell Model Problem for Zr Isotopes

Any reliable shell model calculation requires the choice of a sufficiently large model space. Once the space has been fixed, the calculation relies on a good choice of the single-particle basis and of the two-body potential.

We perform shell model calculations 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 dimensions of the shell model Hamiltonian matrix to be diagonalized for the ground state of ^{91}Zr to ^{102}Zr are listed in Table 1. The shell model eigenvalue problem can be solved exactly only for the lightest Zr isotopes. For ^{96}Zr and beyond, a severe truncation of the configuration space is required.

Table 1. Dimension of the shell model problem for the the ground state of the Zr isotopes

Nucleus	J^π	dimension	Nucleus	J^π	dimension
^{91}Zr	$5/2^+$	636 743	^{97}Zr	$1/2^+$	54 311 712 344
^{92}Zr	0^+	9 933 196	^{98}Zr	0^+	162 778 727 590
^{93}Zr	$5/2^+$	87 386 047	^{99}Zr	$1/2^+$	423 647 760 200
^{94}Zr	0^+	640 713 998	^{100}Zr	0^+	901 962 798 918
^{95}Zr	$5/2^+$	3 254 272 514	^{101}Zr	$3/2^+$	1 469 054 147 739
^{96}Zr	0^+	14 872 779 180	^{102}Zr	0^+	2 867 081 318 378

The second crucial ingredient of the shell model calculations is the effective nucleon–nucleon interaction within the chosen configuration space. We use the code of M. Hjorth-Jensen [6] to generate a $G-$matrix starting from the "CD-Bonn" nucleon-nucleon potential.

We are now ready to perform the calculation. To this purpose, we found useful to adopt the modified Hamiltonian:

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

where α is a positive constant. Due to the additional term, the states with total spin different from j are pushed up in energy for a sufficiently large α. Thus, the diagonalization yields only the low-lying states of a given spin j.

The first task is to check the convergence properties of the sampling procedure. From Figure 1, one can see that the eigenvalues of the lowest states with $J^\pi = 0^+$ have a steep exponential trend and reach their asymptotic (exact) values with just a fraction of one percent of the total size of the Hamiltonian. Also the j value is reproduced very accurately.

In order to obtain a reliable description of the properties of complex nuclei like ^{94}Zr we need to search for an optimal set of single particle energy levels. This search will be done by trying to reproduce low-lying spectrum of the ^{91}Zr.

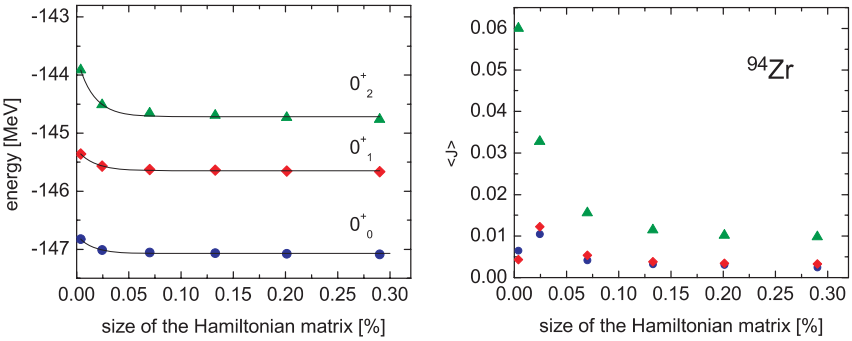

Figure 1. Convergence of the APL results for the energy and the total spin of the ground state and the first two excited 0^+ states in ^{94}Zr. The characteristics of the ground state are denoted by blue dots, for the first two excited 0^+ by red diamonds and green triangles, respectively.

3 Results for ^{91}Zr

The Hamiltonian matrix of ^{91}Zr has a modest dimension (see Table 1) and can be diagonalized exactly. To achieve a better fit of the energy spectrum to the experimental data we allow a scaling factor to the monopole term of the proton-neutron interaction between the proton $1g_{9/2}$ and the neutron $2d_{5/2}$ states as well. The single particle energies obtained by using a scaling factor 1.85 are listed in Table 2.

Table 2. Effective single particle energies for ^{91}Zr in MEV

Protons		Neutrons	
$1f_{5/2}$	-10.16	$2d_{5/2}$	1.12
$2p_{3/2}$	-10.56	$1g_{7/2}$	0.00
$2p_{1/2}$	-8.96	$2d_{3/2}$	0.97
$1g_{9/2}$	-7.43	$3s_{1/2}$	0.05
		$1h_{11/2}$	2.26

The computed low-lying spectrum is shown in Figure 2. The figure shows also the experimental levels and a theoretical spectrum calculated by a method based on Lanczos [7]. This calculation was performed within the same configuration space but with a different effective interaction. It is seen that, by a minimal correction to the effective potential produced by the code of M. Hjorth-Jensen [6], we obtain a very good description of the experimental data for the positive parity states. The excitation energy of the $11/2^-$ state is misplaced in the spectrum and its correct reproduction would require further tuning of the interaction.

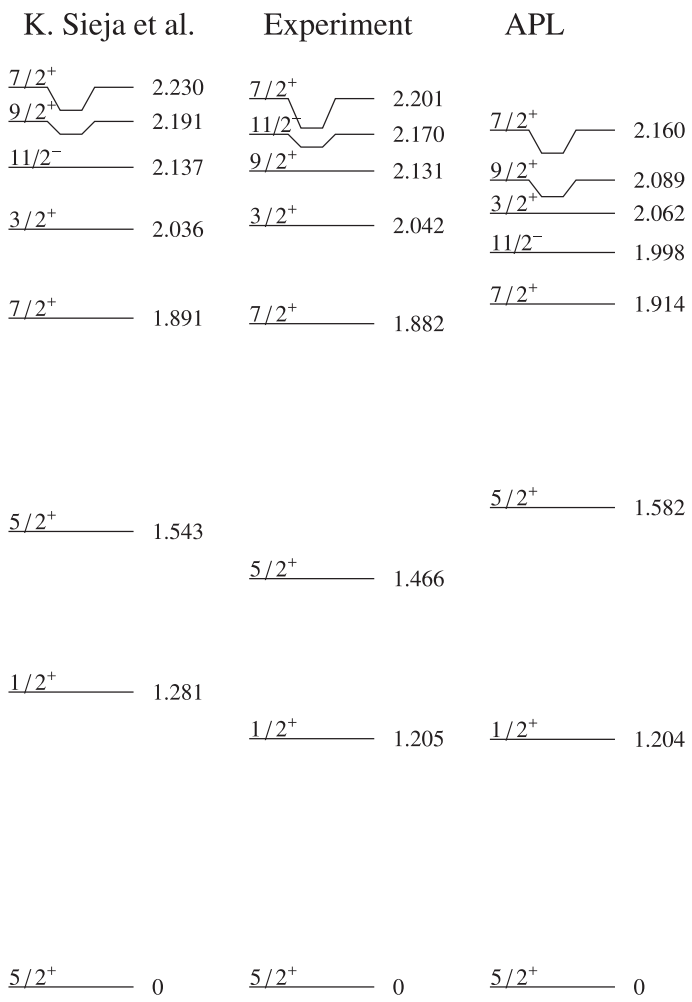

Figure 2. Experimental level scheme of the low-lying energy spectrum of ^{91}Zr [5], compared with the this work's results and those by K. Sieja *et al.* [7].

The gross picture of the nuclear structure of the ground state and the low-lying excited states can be obtained by looking at the occupation numbers of the single particle levels. Their values are listed in Table 3 for the ground state and the first excited states.

It is seen that even in the ground state there is a considerable depletion of the proton Fermi see while the single neutron occupies predominately a single shell.

More detailed insight into the structure of the many–body wave function is provided by the expansion coefficients C_n of the eigenfunction, in terms of Slater determinants, $\Phi = \sum_n C_n \phi^n_{SD}$. The largest C^2_n values for the first three

Table 3. Occupation numbers of the single-particle levels of the ground state and the first excites states in ^{91}Zr

	Protons					Neutrons			
J^π	$5/2^+(g.s.)$	$1/2^+$	$5/2^+$	$7/2^+$	J^π	$5/2^+(g.s.)$	$1/2^+$	$5/2^+$	$7/2^+$
$1f_{5/2}$	5.207	5.428	5.611	5.488	$2d_{5/2}$	0.989	0.015	0.988	0.885
$2p_{3/2}$	3.819	3.890	3.642	3.581	$1g_{7/2}$	0.001	0.001	0.004	0.106
$2p_{1/2}$	1.645	1.737	0.822	0.758	$2d_{3/2}$	0.002	0.003	0.003	0.004
$1g_{9/2}$	1.329	0.943	1.924	2.171	$3s_{1/2}$	0.003	0.976	0.002	0.001
					$1h_{11/2}$	0.004	0.005	0.001	0.001

$5/2^+$ states are seen in Table 4. They show that for all states considered, the neutron occupies the $2d_{5/2}$ level. The proton component of the ground state wave function is dominated by the Slater determinant of lowest energy. The first two excited $5/2^+$ states contain configurations with two protons promoted to the $1g_{9/2}$ level.

Table 4. Slater determinants with largest occupation probabilities in the ground state and the first two excites $5/2^+$ states in the many-body wave function of ^{91}Zr

SD configuration	$5/2^+_{g.s.}$	$5/2^+_2$	$5/2^+_3$
$\nu:\ d^1_{5/2}$ $\pi:\ f^6_{5/2}\ p^4_{3/2}\ p^2_{1/2}$	**0.7388**	7.083E-2	9.689E-3
$\nu:\ d^1_{5/2}$ $\pi:\ f^6_{5/2}\ p^4_{3/2}\ g_{9/2}\ g_{-9/2}$	2.228E-2	**0.2547**	5.885E-3
$\nu:\ d^1_{5/2}$ $\pi:\ f^6_{5/2}\ p^4_{3/2}\ g_{7/2}\ g_{-7/2}$	1.516E-2	**0.1134**	6.512E-4
$\nu:\ d^1_{5/2}$ $\pi:\ f^6_{5/2}\ p^4_{3/2}\ g_{1/2}\ g_{-1/2}$	9.226E-3	1.545E-2	**0.1103**

4 Conclusions

This contribution is the first status report of the project aiming to study the properties of the Zr isotopes within the large–scale shell model. We employed the APL diagonalization algorithm [1, 2] and made use of the important sampling in order to truncate the configuration space. We have reported results about the energies of the low-lying excited states and the occupation numbers of the shell model single–particle levels for ^{91}Zr. We found that the calculation reproduces the experimental energy spectrum with good accuracy by a slight modification of the monopole component of the effective potential.

These first results encourage us ro proceed further by a systematic and thorough study of the spectra and electromagnetic properties of the even Zr isotopes.

Acknowledgements

We would like to thank Morten Hjorth-Jensen for the helpful discussion on generating an effective nucleon-nucleon interaction. S.S.Dimitrova is grateful to Istituto Nazionale di Fisica Nucleare (INFN) for the financial support and the Dipartimento di Scienze Fisiche, Università di Napoli Federico II for the warm hospitality. This work is partly supported by the grants D-02-285 of the Bulgarian Science Fond.

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