EXPONENTIAL CONVERGENCE METHOD AT WORK

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Shell-model calculations of the ground state and low-lying excited states are essential for our understanding of nuclear dynamics and the (effective) nuclear forces. The nuclear shell model with the effective two-body interactions in a restricted Hilbert space is the best available theoretical tool for calculating the properties of the low-lying states. The region of the nuclear chart between Ca and Ni is especially important for coming radioactive beam experiments and astrophysical applications. However, full shell-model calculations are being limited by the exponential increase of the dimension of the many-body Hilbert space with the number of valence nucleons. In the past decade, several approximate methods were proposed to deal with the dimensionality problem. Below we apply the Exponential Convergence Method (ECM) [1].

In the ECM, possible configurations of valence nucleons in the finite number of single-particle states are ordered according to their centroid energies. In a truncation scheme [2] for the low-lying states, higher configurations can be consecutively added to the many-body model space in order of their centroid values. It was shown in Ref. [1] that, as a function of the dimension of truncated Hilbert space, the energies of the low-lying states converge exponentially to their exact values. The physics underlying this numerical observation is associated with the exponentially decreasing admixtures of energetically distant configurations both in the realistic shell model and in random matrices. Being analogous to the exponential localization of coordinate wave functions of electronic states in disordered solids, the same physics is revealed in the exponential behavior of the remote energy tails of the strength functions of simple states in complex atoms and nuclei. The strict mathematical arguments were developed for tridiagonal matrices [1]. This property of exponential convergence can be successfully used to predict the exact energy of the many-body eigenstates. According to Ref. [2], the initial truncation size should exceed a certain value related to the spreading width of typical basis states found from the Hamiltonian matrix prior to its diagonalization. It was also suggested that the matrix elements of observables can be extracted by a similar procedure.

Here we developed the ECM into a practical tool and calculated energies, spins and isospins of the ground states for the nuclei from ^{42}Sc to ^{56}Ni. We performed the calculation for the nuclides having the lowest isospin projection (0 for even A, and 1/2 for odd A) because they include the largest amount of correlations for a given number of valence nucleons. We use the FPD6 interaction [3] which was designed to describe accurately nuclei with $A = 44 - 46$, and it is known to better describe the energy gaps around ^{56}Ni. The results for the calculated ground-state energies and quantum numbers $J^\pi T$ are summarized in Table I. In all cases but one, the experimental spin J is correctly reproduced. The only exception is for $A = 45$, where the three lowest states with spins $J = 3/2, 5/2$, and 7/2 are nearly degenerate within 100 keV both in theory and experiment. Parities and isospins (when available) are always reproduced correctly. The m-scheme dimensions are listed in Table II along with the dimensions of the JT space corresponding to the ground-state quantum numbers. Energies of the nuclei up to $A = 49$ (less than 10 valence nucleons) were calculated using full shell-model spaces; for $A > 49$ the ECM was used. The ground-state energy for ^{56}Ni, -203.280 MeV, is about 200 keV lower than the recently reported value [4] derived by the Quantum Monte Carlo Diagonalization Method. A similar study using the code NATHAN [5] and the KB3 interaction was recently reported but $A = 53$ and 55 nuclei were not calculated.

A	Nuclei	$E_{\rm g.s.}$(SM)	$E_{\rm g.s.}$(exp)	$J^\pi T$	$(J^\pi T)_{\rm exp}$
42	^{42}Sc	-19.814	-20.026	$0^+\ 1$	$0^+\ 1$
43	^{43}Sc	-32.104	-32.115	$7/2^-\ 1/2$	$7/2^-\ 1/2$
44	^{44}Ti	-48.142	-48.381	$0^+\ 0$	$0^+\ 0$
45	^{45}Ti	-57.782	-57.453	$3/2^-\ 1/2$	$7/2^-\ 1/2$
46	^{46}V	-70.696	-71.009	$0^+\ 1$	$0^+\ 1$
47	^{47}V	-83.936	-83.864	$3/2^-\ 1/2$	$3/2^-\ 1/2$
48	^{48}Cr	-99.970	-100.030	$0^+\ 0$	$0^+\ 0$
49	^{49}Cr	-110.029	-110.416	$5/2^-\ 1/2$	$5/2^-\ 1/2$
50	^{50}Mn	-122.400	-123.292	$0^+\ 1$	$0^+\ 1$
51	^{51}Mn	-135.340	-136.734	$5/2^-\ 1/2$	$5/2^-\ 1/2$
52	^{52}Fe	-150.980	-152.631	$0^+\ 0$	$0^+\ 0$
53	^{53}Fe	-160.880	-163.020	$7/2^-\ 1/2$	$7/2^-\ 1/2$
54	^{54}Co	-173.800	-176.114	$0^+\ 1$	$0^+\ 1$
55	^{55}Co	-187.000	-189.861	$7/2^-\ 1/2$	$7/2^-\ 1/2$
56	^{56}Ni	-203.280	-205.992	$0^+\ 0$	$0^+\ 0$

Table I: Theoretical and experimental ground state energies (in MeV), spins and isospins.

In the ECM, each consecutive truncation step includes new shell-model partitions (with increasing energy centroids) in their entirety. For small dimensions, the decrease of the truncated ground-state energy is faster than exponential. This behavior can be attributed to a relatively coherent contribution of the lowest centroid configurations to the structure of the ground state as compared to more chaotic contributions of the high centroid configurations. It is important to have a working recipe for approximating the dimension where the exponential behavior starts. In the last column of Table II we include the ratio $(E_s - E_m)/\sigma$, where E_s is the centroid energy of the configuration at which the exponential behavior starts, E_m is the lowest centroid energy, and σ is the width of the lowest configuration. We observe, in agreement with [2], the exponential behavior starting at a configuration whose centroid energy is 3-4 σ above that for the lowest energy configuration.

A	Nuclei	JT dim	m-scheme dim	$(E_s - E_m)/\sigma$
42	^{42}Sc	4	60	
43	^{43}Sc	61	472	
44	^{44}Ti	66	4000	
45	^{45}Ti	1250	21691	
46	^{46}V	1514	121440	3.0
47	^{47}V	18392	483887	2.9
48	^{48}Cr	9741	1963461	3.1
49	^{49}Cr	232514	6004205	3.3
50	^{50}Mn	134361	18600516	3.2
51	^{51}Mn	1417374	44993824	3.2
52	^{52}Fe	671159	109954620	3.2
53	^{53}Fe	7008147	214688113	3.5
54	^{54}Co	2299178	422818560	3.9
55	^{55}Co	19950699	675477701	4.0
56	^{56}Ni	2581576	1087455228	4.0

Table II: Dimensions of the JT-projected basis corresponding to the ground-state quantum numbers (see Table I), and maximum m-scheme dimensions.

In order to compare the ground-states energies in Table I with experiment, one must correct the experimental values relative to the core of ^{40}Ca for Coulomb effects:

$$H_C = \epsilon_\pi N_\pi + V_{\pi\pi}\frac{N_\pi(N_\pi-1)}{2} + V_{\pi\nu}N_\pi N_\nu. \quad (1)$$

Here $N_\pi(N_\nu)$ denotes a number of valence protons (neutrons), and the following values of the parameters were used [5]: $\epsilon_\pi = 7.440$ MeV, $V_{\pi\pi} = 0.274$ MeV, $V_{\pi\nu} = -0.049$ MeV. They were obtained [5] by fitting the Coulomb displacement energies for analog nuclei between $A = 42$ and $A = 64$.

Table I presents theoretical and experimental ground-state energies of all considered nuclei relative to the core of ^{40}Ca. The general agreement seems to be good, however, toward $A = 56$ the binding energy predicted by the FPD6 interaction is slightly smaller than the experimental value. Following Ref. [5], the simplest correction we can make is to add monopole terms to the single-particle energies and matrix elements of the FPD6 interaction in a form that does not change the wave functions:

$$E(\mathrm{theo}) = E(\mathrm{SM}) + E_{\mathrm{monopole}}\ , \quad (2)$$

where

$$E_{\mathrm{monopole}} = en + \frac{1}{2}n(n-1)v\left(\frac{42}{n+42}\right)^{0.35}. \quad (3)$$

Here $n = A - 40$ is the number of valence nucleons in the fp shell, e is the one-body monopole contribution to average single-particle energy of the major shell, v is the average monopole contribution to the two-body matrix elements. The mass dependence in the equation is the same as that assumed for the FPD6 interaction. The overall quality of the resulting fit is very good; the mean square deviation is 0.27 MeV.

Full fp calculations of the ground state energies of $A = 43$ and $A = 45$ nuclei are reported, to our knowledge, for the first time. The results indicate that the ECM is a powerful tool for calculating the properties of low-lying states when the full large-scale shell-model diagonalization is not feasible. The FPD6 interaction with monopole corrections can be successfully used to describe the ground-state properties of the fp nuclei. Additional studies along the same line for the excited states, transition probabilities and other observables are necessary.

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