Large-Scale Shell-Model Challenges within the RIB Era

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Abstract

In this contribution, we present a procedure that aims to reduce the computational complexity of large-scale shell-model calculations by taking into account the rejected degrees of freedom in an effective approach. Starting from a general large-scale shell-model Hamiltonian, the study of the behavior of its effective single-particle energies as a function of the number of valence nucleons, allows to establish a reduced model space made up only by orbitals needed to describe a certain class of isotopes or isotones. Next, an unitary transformation of the original Hamiltonian is performed from its model space into the truncated one. By virtue of this transformation, a new shell-model Hamiltonian is obtained, which is defined in a smaller model space preserving effectively the role of the excluded single-particle orbitals. As an application of this procedure, we present the results obtained for Mo isotopes outside the ^{88}Sr core, starting from shell-model Hamiltonians derived by way of the many-body perturbation theory from a realistic nucleon-nucleon potential. We present also a study of the dependence of shell-model results upon different truncations of the original model spaces, in order to demonstrate the reliability of this truncation procedure.

Keywords: *Nuclear shell model; realistic nucleon-nucleon potentials; effective interactions*

1 Introduction

The nuclear many-body problem is far more computationally complex than other physical many-body problems because of the nature of the nuclear force. The latter is responsible for correlations between the constituent particles of the nuclei which are stronger than the corresponding ones in atomic and molecular systems, giving a hard life to nuclear microscopic models that take into account single-particle (SP) degrees of freedom of the nucleons.

Recent advances in computer technology have stimulated the development of *ab initio* nuclear structure models which have extended their range of application from light- to medium-mass nuclei.

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For heavier mass nuclei, the nuclear shell model (SM) is still the most profitable approach to the description of nuclei in terms of microscopic degrees of freedom of the valence nucleons with respect to the inert core.

As mentioned before, high-performance computing devices are widely accessible and the SM calculations with large model spaces and for nuclear systems with many valence nucleons are becoming more feasible. These large-scale shell-model (LSSM) calculations are at present a formidable tool to describe the collective properties of atomic nuclei within a microscopic approach and a sound support of experimental efforts aimed to improve the knowledge of the chart of the nuclides in the rare-ion-beam era.

In this regard, it is worth to mention, among many works, the study of the onset of collectivity at $N = 40$ [1], the revelation of a novel shape evolution in nickel isotopes [2], the merging of the islands of inversion at $N = 20$ and $N = 28$ [3], the description of shell evolution leading to the quenching of the $N = 82$ shell gap near ^{120}Sr [4].

However, there exists always an upper limit to the dimension of matrices that have to be diagonalized to solve the SM eigenvalue problem, in spite of the progress in the computer technology. Consequently, most of the LSSM calculations need to introduce some truncation of the SM basis in order to compute theoretical quantities.

In Ref. [1], in order to study the observed onset of collectivity at $N = 40$ in the chromium and iron isotopic chains, a LSSM calculation has been performed employing a model space spanned by the four fp proton orbitals and five $fpgd$ neutron ones, with 4 and 6 valence protons and up to 12 valence neutrons. In order to diagonalize the SM Hamiltonian using the NATHAN code [5], the authors have truncated the basis including up to$= 14p{-}14h$ excitations across the $Z = 28$ and $N = 40$.

The appearance of the shape coexistence in low-energy states of nickel isotopes [2] has been investigated in terms of the SM considering both proton and neutron model spaces spanned by six orbitals $0f_{7/2}, 1p_{3/2}, 1p_{1/2}, 0f_{5/2}, 0g_{9/2}, 1d_{5/2}$ outside the doubly-closed ^{40}Ca core. In the m-scheme the dimension of the basis is $\simeq 10^{24}$, so in Ref. [2] it has been resorted to the importance sampling of the SM states performed within the Monte Carlo Shell Model (MCSM) approach to reduce the matrix dimension to 50 [6].

The $N = 20$ and $N = 28$ islands of inversion have been described by the LSSM calculations within the full $sdpf$ model space [3], but the basis has been restricted so that only the neutron $N = 20$ cross-shell excitations have been taken into account. In such a case, the SM basis has a dimensionality of up to 10^{10}.

In Ref. [4], the authors aim to study the evolution of the neutron $N = 82$ shell gap along the isotonic chain by way of the LSSM calculations. They have employed a model space spanned by proton orbitals $0f_{5/2}, 1p_{3/2}, 1p_{1/2}, 0g_{9/2}, 0g_{7/2}, 1d_{5/2}$, and 7 neutron orbitals $0g_{7/2}, 1d_{5/2}, 1d_{3/2}, 2s_{1/2}, 0h_{11/2}, 1f_{7/2}, 2p_{3/2}$, which allow core excitations across both the $N = 82$ neutron and $Z = 50$ proton shell gaps. In such a case, the diagonalization of the SM Hamiltonian could be performed only by truncating the basis so to allow only one valence-neutron in the $1f_{7/2}, 2p_{3/2}$ neutron orbitals.

These examples show how the calculations for nuclei with many valence nucleons — within large model spaces — are very demanding from the computational point of view, and oblige the researchers in many situations to employ some truncation of the SM basis.

However, whenever the number of valence particle increases, we should consider

also an evolution of theoretical effective SP energies (ESPE) of the SM Hamiltonian.

This evolution of the behavior of the ESPE as a function of the number of valence protons or neutrons may be helpful to locate the relevant degrees of freedom to describe the spectroscopy of a class of isotopes or isotones, and consequently to provide a criterion to reduce the degrees of freedom of the model space.

In a recent work [7], we have proposed a method, already employed in Ref. [8], to perform a very effective truncation of the model space, based on the study of the ESPE of the SM Hamiltonian H as a function of Z_{val} and/or N_{val}. Next, a new SM Hamiltonian $\tilde{H}$ defined in a reduced model space with a smaller number of orbitals, is built up through an unitary transformation of the "mother Hamiltonian" H.

Here, as an application of this method, we will report some results obtained for Mo isotopes outside the closed-shell nucleus ^{88}Sr.

The "mother Hamiltonian" H is derived from the CD-Bonn potential [9], whose high-momentum repulsive components are smoothed out using the $V_{\rm low-k}$ approach [10], utilizing the time-dependent perturbation theory [11]. This will be done within a large model space that includes seven *psdgh* proton and five *sdgh* neutron orbitals.

At the following step, the behavior of the proton and neutron ESPE as a function of the number of valence neutrons and protons is analyzed. The study of the ESPE suggests how to reduce the number of proton and neutron orbitals. After this, we derive — by means of a unitary transformation of the starting SM Hamiltonian — new effective Hamiltonians defined in the reduced model spaces and tailored to study specific isotopic chains. Finally, the SM calculations with these effective Hamiltonians are performed and the theoretical results are compared.

In the following Section, we present some details about the derivation of our shell-model Hamiltonians and effective charges of the electric quadrupole operators, and how we derive the new effective Hamiltonians within the truncated model spaces. In Section 3, we report the results of our calculations for Mo isotopes starting from different model spaces. Finally, we summarize our results in the final Section.

2 Outline of calculations

The first step in our procedure is the derivation from the CD-Bonn NN potential [9] of a starting effective SM Hamiltonian in the framework of the many-body perturbation theory. More explicitly, we first renormalize high-momentum repulsive components of the bare NN potential using the so-called $V_{\rm low-k}$ approach [10], which provides a smooth potential preserving exactly the on-shell properties of the original NN potential up to a cutoff momentum $\Lambda = 2.6$ fm^{-1}. Next, the SM Hamiltonian is derived using the well-known $\hat{Q}$-box plus folded-diagram method, where the $\hat{Q}$-box is a collection of irreducible valence-linked Goldstone diagrams which we calculate through the third order in the $V_{\rm low-k}$ [11].

The effective Hamiltonian $H_{\rm eff}$ can be written in an operator form as

$$H_{\rm eff} = \hat{Q} - \hat{Q}' \int \hat{Q} + \hat{Q}' \int \hat{Q} \int \hat{Q} - \hat{Q}' \int \hat{Q} \int \hat{Q} \int \hat{Q} \; + \; \ldots , \qquad (1)$$

where the integral sign represents a generalized folding operation, and $\hat{Q}'$ is obtained from $\hat{Q}$ by removing the terms of the first order in $V_{\rm low-k}$. The folded-diagram series is summed up to all orders using the Lee–Suzuki iteration method [12].

The effective Hamiltonian $H_{\rm eff}$ provides both the SP energies and two-body matrix elements of the residual interaction [11], and we can derive consistently, within the same perturbative approach, the effective operators $\hat{O}_{\rm eff}$ (e. g., electromagnetic operators, Gamow–Teller transition operator) whose effects we want to study.

Both $H_{\rm eff}$ and $\hat{O}_{\rm eff}$ are defined in a large model space labelled $[N_p, N_n]$, where N_p and N_n are the numbers of proton and neutron orbitals spanning the model space, respectively. Therefore, for the sake of clarity, we dub the effective Hamiltonian and the effective operators as $H^{N_pN_n}$ and $\hat{O}^{N_pN_n}$.

As mentioned in the Introduction, in the case of large model spaces, the major computational difficulties arise when evolving the number of the valence protons Z_{val} (isotonic chains) and/or of the valence neutrons N_{val} (isotopic chains) makes the calculation unfeasible with up-to-date SM codes. It is then mandatory to reduce the complexity of the SM problem to be solved.

In the following we describe an approach that we have adopted with success in Refs. [7, 8], which leads to new effective Hamiltonians defined in truncated model spaces by way of a unitary transformation of $H^{N_pN_n}$. The choice of the truncated model space, $[n_p, n_n]$, is driven by the analysis of the behavior, as a function of Z_{val} and N_{val}, of the proton and neutron ESPE of the original Hamiltonian $H^{N_pN_n}$ so as to find out what are the most relevant degrees of freedom to describe the physics of nuclear systems of interest.

Here we describe the derivation of the new SM effective Hamiltonian $H^{n_pn_n}$ starting from the "mother Hamiltonian" $H^{N_pN_n}$.

The eigenvalue problem for $H^{N_pN_n}$ can be written in terms of its eigenvalues E_i and eigenfunctions ψ_i,

$$H^{N_pN_n}|\psi_i\rangle = E_i|\psi_i\rangle, \tag{2}$$

where $H^{N_pN_n}$ may be expressed as the sum of a SP Hamiltonian H_0 and a residual two-body potential V:

$$H^{N_pN_n} = H_0 + V. \tag{3}$$

As it has been mentioned before, the analysis of the behavior of the ESPE induces a possible reduction of the number SP orbitals that span the model space. The original model space $[N_pN_n]$ is then split up into two subspaces defined by the projectors $P \equiv P^{n_pn_n}$ and $Q \equiv Q^{N_p-n_p,N_n-n_n}$, with the projector P expressed in terms of the H_0 eigenvectors

$$P = \sum_{i=1,d} |i\rangle\langle i|, \qquad H_0|i\rangle = E_i^0|i\rangle. \tag{4}$$

The P-space effective Hamiltonian $H^{n_pn_n}$ is defined by the equation

$$H^{n_pn_n}|\phi_k\rangle = (PH_oP + V^{n_pn_n})\,|\phi_k\rangle = E_k|\phi_k\rangle, \tag{5}$$

where we require that the eigenfunctions ϕ_k are the projections of the eigenfunctions ψ_k of the "mother Hamiltonian",

$$|\phi_k\rangle = P|\psi_k\rangle.$$

Formally, we can express $H^{n_pn_n}$ as

$$H^{n_pn_n} = \sum_{k=1}^{d} E_k|\phi_k\rangle\langle\tilde{\phi_k}|, \tag{6}$$

where $|\tilde{\phi_k}\rangle$ are the $|\phi_k\rangle$ biorthogonal states satisfying $|\tilde{\phi_k}\rangle\langle\phi_{k'}| = \delta_{kk'}$ and obtained using the Schmidt biorthonormalization procedure.

The effective residual interaction $V^{n_p n_n}$ can therefore be expressed as

$$V^{n_p n_n} = \sum_{k=1}^{d} E_k |\phi_k\rangle\langle\tilde{\phi_k}| - PH_0P. \tag{7}$$

The knowledge of the eigenvalues and eigenfunctions of $H^{N_p N_n}$ is therefore essential to derive explicitly the effective Hamiltonian $H^{n_p n_n}$.

Let us now briefly describe the derivation of the P-space effective operator $\hat{O}^{n_p n_n}$. By definition, $\hat{O}^{n_p n_n}$ has to satisfy the following condition

$$\langle\Psi_k|\hat{O}^{N_p N_n}|\Psi_{k'}\rangle = \langle\tilde{\phi_k}|\hat{O}^{n_p n_n}|\phi_{k'}\rangle, \tag{8}$$

where $\hat{O}^{N_p N_n}$ is the operator defined in the starting large model space. By analogy with what we have done for the Hamiltonian, we can express $\hat{O}^{n_p n_n}$ formally as

$$\hat{O}^{n_p n_n} = \sum_{\alpha,\beta=1}^{d} \langle\Psi_\alpha|\hat{O}^{N_p N_n}|\Psi_\beta\rangle|\phi_\alpha\rangle\langle\tilde{\phi_\beta}|. \tag{9}$$

It can be easily shown that the above expression satisfies Eq. (8). The knowledge of the $\langle\Psi_k|\hat{O}^{N_p N_n}|\Psi_{k'}\rangle$ matrix elements is therefore essential for the explicit derivation of the effective operator $\hat{O}^{n_p n_n}$.

It is worth to point out that when solving the $H^{N_p N_n}$ eigenvalue problem for a A_{val} valence-nucleon system, the corresponding effective Hamiltonian $H^{n_p n_n}$ and effective operator $\hat{O}^{n_p n_n}$ contain 1-body, 2-body, ... , A_{val}-body contributions. To our knowledge, however, there are no public SM codes able to handle either these n-body forces with $n \geq 3$ or the effective operator n-body contributions with $n \geq 2$. Therefore, we have applied the above transformation only to the two valence-nucleon systems, thus obtaining only two-body matrix elements of $H^{n_p n_n}$, while we have taken into account only the one-body component of $\hat{O}^{n_p n_n}$.

3 Results of SM calculations

As already mentioned in the Introduction, we considered for calculations outside the ^{88}Sr core the model space spanned by seven proton $1p_{1/2}$, $0g_{9/2}$, $0g_{7/2}$, $1d_{5/2}$, $1d_{3/2}$, $2s_{1/2}$, $0h_{11/2}$ and five neutron $0g_{7/2}$, $1d_{5/2}$, $1d_{3/2}$, $2s_{1/2}$, $0h_{11/2}$ orbitals. Hereafter this model space will be labelled [75]. In accord with notations introduced in the previous Section, the respective SM effective Hamiltonian is dubbed H^{75}, the superscript referring to the number of proton (seven) and neutron (five) model-space orbitals. This large model space is able to take explicitly into account the $Z = 50$ cross-shell excitations of protons jumping from the $1p_{1/2}$, $0g_{9/2}$ orbitals to the *sdgh* ones.

We report in Table 1 the calculated SP energies and in Table 2 the theoretical proton and neutron effective charges, the latter being close to the usual empirical values ($e_p^{\rm emp} = 1.5e$, $e_n^{\rm emp} = 0.5{-}0.8e$).

The trouble with the SM Hamiltonian H^{75} is the computational complexity which arises when the atomic number Z of the isotopic chain under investigation is evolved.

Table 1: Theoretical SM SP energy spacings (in MeV) (see text for details).

nlj	proton SP energies	neutron SP energies
$1p_{1/2}$	0.0	
$0g_{9/2}$	1.5	
$0g_{7/2}$	5.7	1.5
$1d_{5/2}$	6.4	0.0
$1d_{3/2}$	8.8	3.4
$2s_{1/2}$	8.7	2.2
$0h_{11/2}$	10.2	5.1

Table 2: Proton and neutron effective charges of the electric quadrupole operator $E2$.

$n_a l_a j_a$	$n_b l_b j_b$	$\langle a\|\|e_p\|\|b\rangle$	$\langle a\|\|e_n\|\|b\rangle$
$0g_{9/2}$	$0g_{9/2}$	1.53	
$0g_{9/2}$	$0g_{7/2}$	1.58	
$0g_{9/2}$	$1d_{5/2}$	1.51	
$0g_{7/2}$	$0g_{9/2}$	1.77	
$0g_{7/2}$	$0g_{7/2}$	1.84	1.00
$0g_{7/2}$	$1d_{5/2}$	1.84	0.98
$0g_{7/2}$	$1d_{3/2}$	1.86	0.98
$1d_{5/2}$	$0g_{9/2}$	1.59	
$1d_{5/2}$	$0g_{5/2}$	1.73	0.92
$1d_{5/2}$	$1d_{5/2}$	1.73	0.87
$1d_{5/2}$	$1d_{3/2}$	1.71	0.90
$1d_{5/2}$	$2s_{1/2}$	1.76	0.73
$1d_{3/2}$	$0g_{7/2}$	1.83	0.94
$1d_{3/2}$	$1d_{5/2}$	1.79	0.93
$1d_{3/2}$	$1d_{3/2}$	1.81	0.92
$1d_{3/2}$	$2s_{1/2}$	1.83	0.75
$2s_{1/2}$	$1d_{5/2}$	1.73	0.73
$2s_{1/2}$	$1d_{3/2}$	1.73	0.73
$0h_{11/2}$	$0h_{11/2}$	1.89	0.87

For example, this Hamiltonian cannot be diagonalized for any tin isotope with up-to-date SM codes.

In order to apply the procedure reported in Section 2, we study the evolution of both proton and neutron ESPE as a function of Z_{val} which are reported in Figs. 1 and 2.

In Fig. 1, it can be observed that a well-defined separation between the proton subspaces $[1p_{1/2}, 0g_{9/2}, 1d_{5/2}, 0g_{7/2}]$ and $[2s_{1/2}, 1d_{3/2}, 0h_{11/2}]$ is provided by an almost

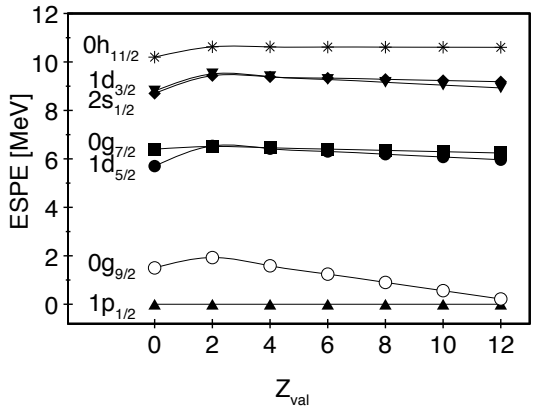

Figure 1: Calculated proton ESPE of H^{75} as a function of the number of valence protons Z_{val}.

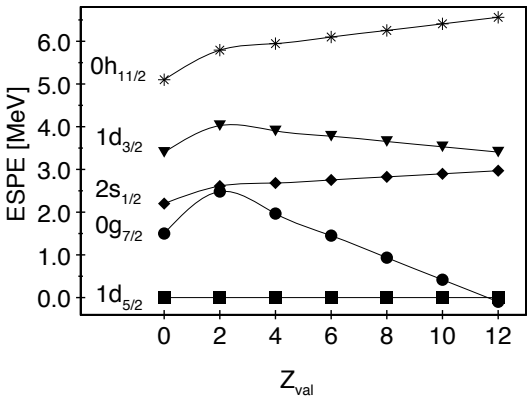

Figure 2: Calculated neutron ESPE of H^{75} as a function of the number of valence protons Z_{val}.

constant energy gap, leading to the conclusion that we can truncate the proton model space to the lowest four orbitals only.

On the neutron side, Fig. 2 evidences that the filling of the proton $0g_{9/2}$ orbital induces a relevant energy gap at $Z = 50$ between the $[1d_{5/2}, 0g_{7/2}]$ subspace and the $[2s_{1/2}, 1d_{3/2}, 0h_{11/2}]$ one. On the above grounds, it looks reasonable to investigate the neutron model space spanned only by the $1d_{5/2}$ and $0g_{7/2}$ orbitals.

Following the procedure reported in Section 2, we have derived two new effective Hamiltonians $H^{45}_{\rm eff}$ and $H^{42}_{\rm eff}$ defined within two model spaces [45] and [42] consisting of the proton $1p_{1/2}$, $0g_{9/2}$, $1d_{5/2}$, $0g_{7/2}$ and of the neutron $0g_{7/2}$, $1d_{5/2}$, $1d_{3/2}$, $2s_{1/2}$, $0h_{11/2}$ and $0g_{7/2}$, $1d_{5/2}$ orbitals, respectively. To verify the reliability of our truncation scheme, we consider the Mo isotopes, more precisely ^{92,94,96}Mo, whose Hamiltonians may be diagonalized within the $[7, 5]$ model space.

In Fig. 3 we compare the absolute energies of yrast $J = 0^+$, 2^+, 4^+ states in ^{92,94,96}Mo obtained by means of the above mentioned effective SM Hamiltonians. It can be noted that both $H^{45}_{\rm eff}$ and $H^{42}_{\rm eff}$ are able to reproduce quite well the absolute energies of the "mother Hamiltonian" H^{75}.

It should be also pointed out that, for ^{96}Mo, $H^{42}_{\rm eff}$ reproduces nicely the 2^+ excitation energy but underestimates the collectivity predicted by the "mother Hamiltonian". In fact, the $R_{4/2}$ ratio between the calculated excitation energies of the 4^+ versus 2^+ states equal to 2.0 with H^{75} and $H^{45}_{\rm eff}$, drops to 1.6 when evaluated with $H^{42}_{\rm eff}$. As a matter of fact, from the inspection of Fig. 2, we should not expect the $H^{42}_{\rm eff}$ results to be in a good agreement with those from H^{75} since there is no a clear separation of the model space P from its complement Q for $Z_{val} = 4$ (Mo isotopes).

The above results evidence the adequacy of our truncation scheme when it is grounded on a neat separation of the model space P from its complement Q as depicted by the ESPE behavior (see Figs. 1 and 2).

As regards the calculation of the $E2$ transition rates using the effective charges derived consistently from the theory, we obtain, for ^{92}Mo, $B(E2; 2^+_1 \to 0^+_1) = 148$ e^{2}fm^4 with $H^{75}_{\rm eff}$ and 160 e^{2}fm^4 with $H^{45,42}_{\rm eff}$. For ^{94}Mo, the calculated result with $H^{75}_{\rm eff}$ is $B(E2; 2^+_1 \to 0^+_1) = 381$ e^{2}fm^4, 323 e^{2}fm^4 with $H^{45}_{\rm eff}$, and 231 e^{2}fm^4 with $H^{42}_{\rm eff}$. Finally, in the case of ^{96}Mo, $B(E2; 2^+_1 \to 0^+_1) = 487$ e^{2}fm^4 with $H^{75}_{\rm eff}$, 451 e^{2}fm^4 with $H^{45}_{\rm eff}$, and 244 e^{2}fm^4 with $H^{42}_{\rm eff}$. It is evident that a faster degradation of the original $E2$ transition rate reproduction occurs when employing the $[4, 2]$ model space as compared to

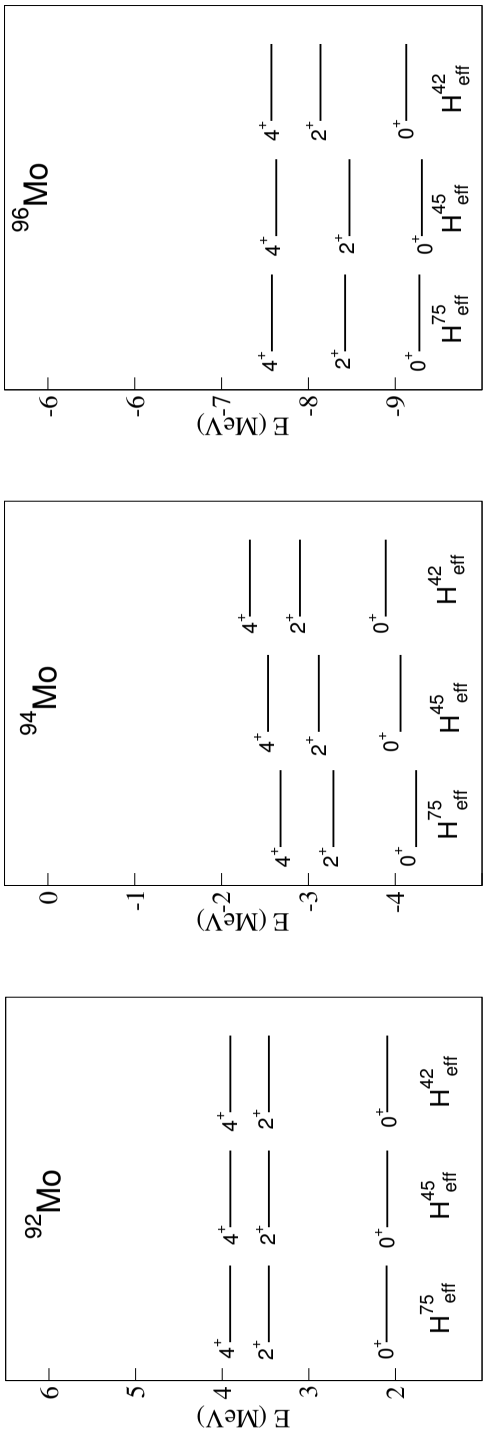

Figure 3: Yrast $J = 0^+, 2^+, 4^+$ states of ^{92,94,96}Mo isotopes calculated within model spaces $[7,5]$, $[4,5]$, and $[4,2]$ (see text for details).

that calculated within the $[7, 5]$ model space.

As pointed out at the end of Section 2, in order to preserve exactly also the calculated transition rates for the two-valence nucleon systems when dealing with the effective Hamiltonians H^{pn}, the effective $E2$ operator should be further renormalized to take into account the neglected degrees of freedom. In this way, one would obtain an effective two-body $E2$ operator to be employed to calculate the electric quadrupole properties of the systems with a number of valence nucleons larger than two. As a consequence, the eventual observed discrepancy between the $E2$ properties calculated with H^{75} and those with the effective Hamiltonians $H^{42}_{\rm eff}$ is a signature of the fact that the corresponding H^{75} wave functions have relevant components outside the truncated [42] model space.

4 Summary

In this paper we have reported on a double-step approach to simplify the computational problem of large-scale SM calculations. The method is based on the study of the ESPE of the large-scale Hamiltonian to identify the most relevant degrees of freedom to be taken into account in the construction of a truncated SM Hamiltonian. To this end, a unitary transformation is employed to derive new effective SM Hamiltonians defined within a reduced set of SP orbitals, accordingly to the ESPE analysis.

This procedure has been applied to a realistic SM Hamiltonian within a model space designed to describe the $Z = 50$ cross-shell excitations for nuclei outside ^{88}Sr by employing seven proton and five neutron orbitals. The behavior of the proton and neutron ESPE allows to identify two truncated model spaces made up by four proton orbitals and five or two neutron ones, and we have transformed our original Hamiltonian in these subsets.

As a test case, we have performed the calculations for Mo isotopes to check the reliability of our procedure. The results obtained with the effectively truncated Hamiltonians testifies the ability to reproduce the eigenvalues and electromagnetic transition rates of the original SM Hamiltonian when the ESPE provide a neat separation in energy between the new model subspaces and their complement.

We are confident that this double-step approach may provide a reliable truncation procedure in any large-scale SM calculation and a theoretical tool that may be applied in other regions where large model spaces lead to critical situations due to the computational complexity, especially when increasing the number of valence nucleons.

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