Model space truncation in shell-model fits

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We carry out an interacting shell-model study of binding energies and spectra in the *sd*-shell nuclei to examine the effect of truncation of the shell-model spaces. Starting with a Hamiltonian defined in a larger space and truncating to the *sd* shell, the binding energies are strongly affected by the truncation, but the effect on the excitation energies is an order of magnitude smaller. We then refit the matrix elements of the two-particle interaction to compensate for the space truncation and find that it is easy to capture 90% of the binding energy shifts by refitting a few parameters. With the full parameter space of the two-particle Hamiltonian, we find that both the binding energies and the excitation energy can be fitted with remaining residual error about 5% of the average error from the truncation. Numerically, the rms initial error associated with our Hamiltonian is 3.4 MeV and the remaining residual error is 0.16 MeV. This is comparable to the empirical error found in *sd*-shell interacting shell-model fits to experimental data [B. A. Brown and W. A. Richter, Phys. Rev. C **74**, 034315 (2006)].

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The interacting shell model with fitted interactions is a powerful predictive tool of nuclear structure theory [1,2], but there has been little study of the error associated with truncation of the shell model spaces. The basic premise is that there exists some Hamiltonian of the nucleon degrees of freedom that accurately describes nuclear structure properties. The interacting shell model is then just a numerical method to calculate the properties of that Hamiltonian. However, except for the lightest nuclei, the spaces that one can include in the calculation are much too small to obtain meaningful results using the full Hamiltonian. The prevailing philosophy for the interacting shell model in heavier nuclei is to use an effective Hamiltonian fitted to the set of nuclei under study. Typically, the effective Hamiltonian includes one- and two-body matrix elements augmented by an overall scaling with mass number A to take into account higher order operators in addition to the known systematic scaling of the rms radius.

In this work we examine the role of space truncation with a model study of spectra in *sd*-shell nuclei. We first define a target Hamiltonian that can be solved in a larger space and take the eigenenergies as the "experimental" data to be fitted. We then carry out the *sd*-shell fits to the target spectra to examine the characteristics of the fitted Hamiltonian.

Methodology. A recent shell-model fit to *sd*-shell nuclei has been carried out by Brown and Richter [3]. The parameters in the effective Hamiltonian are the 3 single-particle energies of the $(d_{5/2}, d_{3/2}, s_{1/2})$ orbitals and their 63 interaction matrix elements. In addition, there is a parameter for the A-dependent scaling of the interaction matrix elements, which is not important for the fit [4]. The experimental data that were fitted were the energies of 608 states in 77 nuclei.

For our model calculations, we shall try to follow Ref. [3] with respect to the size and character of the data set to be fit. We consider the nuclei in the *sd* shell for which $Z \leqslant N$, ranging from ^{17}O to ^{40}Ca. This gives 90 binding energies with respect to the closed ^{16}O core. Besides binding energies, we also include the excitations of the 6 lowest excited states in the spectrum where they exist. When there are fewer states in the *sd* space, e.g., for the nuclei $(Z, N) = (8, 9), (8, 20)$, we take all the states of the spectrum. Altogether, we fit 559 excitation energies.

The target values of the energies, simulating the experimental data, are calculated from a shell-model Hamiltonian in an extended space. The choice of the space requires a compromise between having the Hamiltonian be computable with modest computer resources and having a space extension that will systematically affect the properties across the range of nuclei under study.

We will then fit the energies of the large space calculation to Hamiltonian parameters for the small space. There are a number of aspects to the refit. Most obviously, we ask how much the rms residuals of the energy shifts shrink going from the original parameters in the small space to a compete refit of all the shell-model parameters. It is also interesting to see the extent that simple parameters of the interaction can capture the main effects of the shifts. We make this quantitative by considering two simple models of the interaction and asking how the rms residuals shrink using only the parameters in the interaction model for the refit.

The target Hamiltonian. For the target Hamiltonian, we begin with the full *sd* Hamiltonian and extend the space to include all $2\hbar\omega$ excitations into higher oscillator shells. This permits two-particle excitations into the *pf* shell and one-particle excitations into the *sdg* shell. This space is large but still reasonably calculable, with the largest matrix dimension being 50 million.

Within the *sd* shell, the Hamiltonian matrix elements are given by Brown and Richter's USDB (universal *sd*-shell interaction B) [3]; we take the values for $A = 18$ but do not rescale them for different A. For the off-diagonal and the *pfsdg* diagonal matrix elements, we take a contact interaction with different strengths for the spin 0 and 1. The strengths are chosen to roughly fit the largest matrix elements of the USDB interaction. The coefficients of the δ functions are 450

and 300 MeV fm^3 for isospin zero and one, respectively; the integrals are evaluated in harmonic oscillator wave functions with oscillator parameter $\hbar\omega = 10.5$ MeV. The single-particle energies are taken to be 5 MeV for the pf orbitals and 10 MeV for the sdg orbitals, taken with respect to zero energy in the USDB Hamiltonian. These energies are smaller than Hartree-Fock single-particle energies, but the empirical spectroscopy of intruder states, namely the typical excitation energy of odd-parity state, requires a substantial reduction of them.

The quantities to be fitted are the differences in energies of the USDB Hamiltonian and the extended-space Hamiltonian. One technical difficulty is ensuring that corresponding states in the two Hamiltonians are properly paired. Furthermore, in some nuclei there are intruder states in the extended-space spectrum that lie below the states that should be paired. The intruders are identified by examining the occupation probabilities of the higher shells removed before making a correspondence with the sd-space levels. The fraction of pf and sdg components is generally between a few percent up to about 20–30% with our interaction. The two states that exceeded this had probabilities greater than 80%, permitting an unambiguous identification as intruders. They were excluded from the spectra to be fitted. Carrying out this procedure, we find that the rms energy differences of the full data sets is 3.4 MeV. Considering binding energies and excitation energies separately, the rms differences are 9.2 and 0.53 MeV, respectively.

Least-squares fit. We then fit the energy differences found in the last section using the 63 matrix elements of the two-particle interaction as fitting parameters. The single-particle energies have the same values in both Hamiltonians and may be directly extracted from the energies of the one-particle nucleus. Those energies were kept fixed in the fits.

In data fitting, it is often the case that some parameters are ill-determined and can assume large, unphysical values when one carries out a linear least-squares fitting procedure. The standard remedy is to make a singular value (SV) decomposition of the least-squares sensitivity matrix and monitor the quality of the fit as a function of the rank of the SV decomposition. The results are shown in Fig. 1, with rms averages for binding energy and excitation energy residuals plotted separately. We see that an enormous improvement in the binding energies can be achieved, a factor of 40 of reduction of the rms error with 19 fitting parameters. By comparison, the improvement in excitation energies is quite modest, reducing the rms error by a factor of 2 with the rank 19 SV fit. The quality of the fit becomes similar for binding energies and excitation energies beyond rank 3. The overall improvement in the energies is a factor of 10 at rank 19 and 20 with high-rank fits. However, the high-rank fits can be deceptive because the fitting procedure relies on the Feynman-Hellman theorem to linearize the error matrix. Qualitative information bearing on the linearization approximation may be seen by plotting the rms changes in the interaction parameters as functions of SV rank. This is shown in Fig. 2. One sees that the interaction parameters change by an average of 0.2 MeV for SV rank 19 and spike to 0.45 MeV at rank 63. For a scale, the rms average two-body interaction in the original USDB parametrization

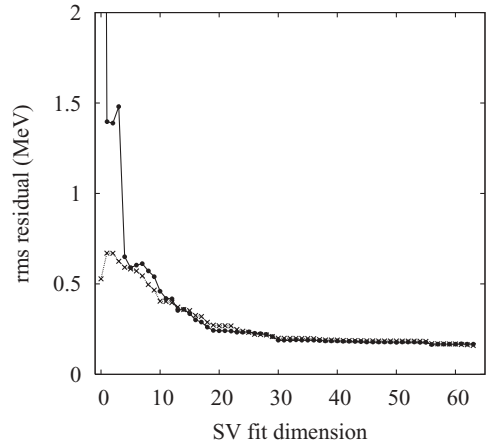

FIG. 1. The rms residual error in the refitted energies as a function of the parameter-space dimension in the singular value decomposition. Solid circles, binding energies; crosses, excitation energies. The initial value of the binding energy residual is off-scale at 9.0 MeV.

is 1.9 MeV, suggesting that the interaction does not become ill-determined, at least up to rank 30 or so. We have confirmed the rank 30 results by rediagonalizing the Hamiltonian matrix using the fitted interaction. The resulting energies have an rms residual only 30% higher than the SV value, confirming the utility of the linear approximation up to that rank.

Simple model Hamiltonians. Because only very few parameters are needed to get the benefit of a refit, the question naturally arises whether the key parameters can be characterized in terms of simple Hamiltonians. For example, it has been found that good results could be obtained by refitting just the monopole part of a realistic interaction [2,5]; this phenomenology has been applied to a number of interactions [6–9] (for details we point the reader to Eqs. (9) and (10) and Appendix B of Ref. [2] and Eq. (4.1) of Ref. [6]). Another possibility, motivated by the Skyrme parametrizations [10,11] and effective field theory [12], is to add an adjustable contact

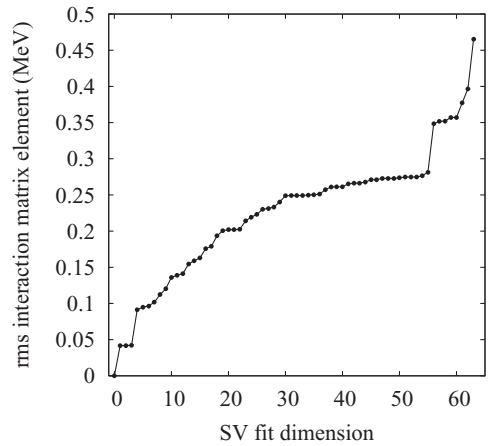

FIG. 2. The rms change in the 63 two-particle interaction matrix element as a function of parameter-space dimension in the singular value decomposition.

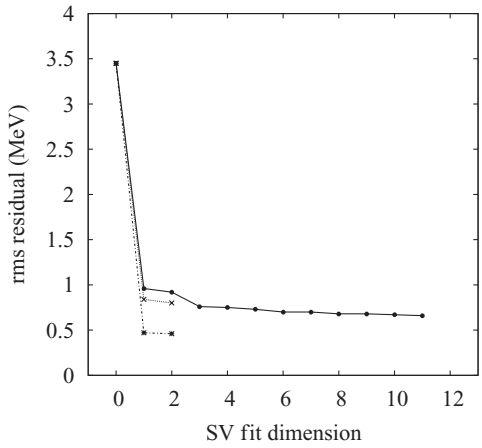

FIG. 3. The rms residual error for simplified forms of the refitted interaction. Solid circles, 12-term monopole interaction; crosses, two-term monopole interaction; stars, two-term contact interaction.

term to the interaction. These two possibilities represent the extremes of very long and very short for the characteristic ranges of the induced interaction. Let us see how well they work.

Monopole interaction. The most general monopole interaction in the *sd* shell has separately adjusted coefficients for the six combinations of subshells as well as for the two isospins ($T = 0$ and 1). The SV fits are shown in Fig. 3 up to rank 11. One sees that the lowest rank captures a very large fraction of the error, and higher ranks make incremental improvements. Asymptotically, the remaining error is 0.7 MeV, which is still four times larger than what can be achieved in the 63-dimensional two-particle matrix elements space. To understand better the nature of the refit producing the large initial error reduction, we have also considered a monopole interaction independent of subshells, i.e., an interaction depending only on particle number. With two terms for the isospin dependence, we find the fits shown by the crosses in the figure. Interestingly, the two-term form gives better fits in the rank 1 and 2 spaces than the full monopole. This can be understood from conjugate gradient methods: the steepest local gradient may in fact not lead to the lowest local minimum.

Contact interactions. There are two ordinary δ-function interactions, depending on spin ($S = 0$ or 1). The results of the fit are shown as stars in Fig. 3 and in Table I. One sees that it is much better than the monopole or the low-rank SV vectors of the full *sd* interaction space.

Conclusion. With our model to study the effects of truncation on the spectra of the interacting shell model, we obtained quite dramatic findings. The energy shifts in the binding energies are more than an order of magnitude larger than those in the excitation energies. The binding energies' shifts can be easily compensated by a one-order two-term interaction of a very simple form, either monopole or contact, with the contact interaction giving a better fit. The importance of the monopole in the SV decomposition of the sensitivity matrix was already shown in Ref. [13]. In that work, the authors considered the entire spectrum of fixed J, T, and A.

TABLE I. The rms residuals (in MeV) in the SV decomposition with various treatments of the parameter fitting.

Interaction	No. of parameters		
	2	11	63
sd two-body	0.80	0.40	0.16
Full monopole	0.92	0.66	
Reduced monopole	0.84		
Contact	0.46		

Our findings are similar, that a single operator close to the monopole dominates the SV decomposition, but the ensemble is very different—all the nuclei are in the Fock space but there are only a few levels in each nucleus.

After a few-parameter fit, the residual errors in the binding energies and the excitation energies are comparable and at the level of 0.5 MeV. Further improvements can be made in the full space of the 63 shell-model matrix elements, with rank 30 achieving a rms residual of 0.2 MeV. We note that the limiting residual in the USDB fit to experimental data [3] is 0.13 MeV.

However, it should be cautioned that these results may depend on the specifics of the Hamiltonian model in the extended space. The overall strength of the off-diagonal interactions cannot be changed very much without either weakening the interaction below what shell systematics require or enhancing it to an extent where many intruder states would seriously contaminate the spectrum. On the other hand, the spin dependence has been very much oversimplified in our model and it could influence the fidelity of the ultimate fit in the small space. For example, it would be interesting to repeat the study including the tensor interaction, which is known to have strong off-diagonal components.

In effective field theory [12], the machinery for performing truncations by the renormalization group is well-developed, with a systematic expansion ordered by counting powers of the relevant momenta, which allows one to estimate the error at a given order of truncation. For the shell-model Hamiltonian, there is no obvious analogy to power counting schemes, although one could argue that SV decomposition provides a logical framework for error estimates. Indeed we have seen that the linear approximation works very well for estimating the change in the residual error. For example, as we go (somewhat arbitrarily) from a rank 10 fit to a rank 30 fit using the SV decomposition, the change in the calculated energies has a rms value of 0.36 MeV, which is within a factor of 3 of the residual error in the complete fit. Besides giving an internal error estimate, such considerations might be helpful in assessing the possible improvements of the fits by going to larger spaces. Finally, it might be interesting to apply such analyses to other many-body approaches, such as energy-density functionals, where one can introduce a very large number of terms beyond the ten or so present in the most familiar parametrizations.

It is intriguing that the error in the fit to experimental data, 0.13 MeV, is actually smaller than the truncation error of our model Hamiltonian, 0.16–0.26 MeV. It might be that the off-diagonal matrix elements in the model Hamiltonian are

too strong. Certainly, the contact interaction has off-diagonal matrix elements larger than those of a more realistic interaction. It also might be the case that the extreme truncation in our model, only allowing $2\hbar\omega$ excitations in higher shells, requires stronger higher-order operators than a more smooth truncation might produce. In any case, the closeness of the limiting error gives some hope that the accuracy of the configuration-interaction theory might be improved by treating the higher shells.

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