

Tutorial on shell model calculations and the production of nuclear Hamiltonians

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I. PROBLEM SET 4

Recall from Problem Sets 1-3 the difficulties with standard interactions and model spaces. Based on Lectures V-VII, you are now able to produce effective interactions from microscopic inputs for calculations beyond standard model spaces.

1. Application to standard model space

- (a) First, evaluate the quality of effective interactions from microscopic interactions by comparing to empirical interactions in a standard model space. Select two stable target nuclei in the *sd* shell. For instance, the core of the model space (^{16}O) and ^{28}Si . Run the 'ham' executable and enter the mass and charge of your first target, then enter the model space ('sdpn'). A batch file has been created to eliminate the hard core (renorm/vrenorm program) and create an effective interaction in a reduced model space (veff/bhf program) with default settings. To speed up the calculation (for the purposes of the tutorial, but not for research purposes), copy the x.inf file to ham.ini. Edit ham.ini to see the default settings. For this application, change both limits on $\hbar\omega$ excitations to 4. Type ham <enter> and a new batch file will be created with the updated settings. Run 'ham' for both target nuclei in this way.¹ Calculation takes approximately 5 minutes for each interaction.
- (b) Compare the two interactions to each other. Consider from Lectures V-VI what is contributing to the difference and evaluate the effect.
- (c) Compare these effective interactions to the empirical USDB interaction.² You do not need to compare every single TBME, but consider the differences in the empirical and microscopic interactions and select appropriate TBME for comparison.
- (d) In addition to comparing TBME directly, perform a comparison of the interactions through full-CI calculations. I recommend calculating the $A = 24$ isobars from Problem Set 1, Problem 1a. You will not need to reproduce the empirical results as the usdb.int interaction in the sd.sp model space produces identical results to the usdbpn.int interaction in the sdpn.sp model space.
- (e) Explain the differences between the empirical and microscopic effective interactions. In part, recall what you learned when you calculated the oxygen isotopes in Problem Set 3, Problem 1a.

2. Application to exotic isotopes

- (a) Recall from Problem Set 1, Problem 4 and Problem Set 3, Problem 2 that the USDB interaction failed for nuclei with $N/Z \approx 2$ near the border of the model space ($N \approx 20$). Select an appropriate model space for calculations of ^{31}Mg and ^{30}Ne .³
- (b) There are multiple correct answers to the prior question, but the supplementary information provides a model space for this question. Create a *.sp file for this model space in proton-neutron formalism, either in the sps folder or in the directory where you will perform calculations. Run the 'ham' executable for the appropriate closed-subshell target nucleus ^{34}Si (recall discussion in Lecture VII). Copy the a_34.inf file to ham.ini and edit ham.ini. Change both limits on $\hbar\omega$ excitations to 4 and select the realistic Skyrme Hartree-Fock basis for spe spectrum and wavefunctions for TBME. Update the batch file by running ham <enter> and then create the effective interaction.

1. Unlike NUSHELLX, which is parallelized with OpenMP and uses all available processors with shared memory, 'ham' is serial. As long as you run the two calculations in different subdirectories (and have two processors on your laptop), you can produce both effective interactions at the same time.

2. I advise you to compare to the usdbpn.int file, which is the USDB interaction in proton-neutron formalism. This way, the ordering of the model space orbits is consistent since they use the same sdpn.sp model space. However, note that the ordering of the TBME is not consistent in the interaction files.

3. Remember that as the model space gets larger, problems can arise with spurious states and divergences in addition to the increasing length of time for calculations. In general, try to select the smallest model space needed to describe the low-energy states of interest.

- (c) Calculate the level schemes of ^{30}Ne and ^{31}Mg and the $B(E2)$ transition from the first excited state to the ground state in ^{30}Ne . Compare to the results with empirical interactions and to experimental data.
- (d) **Optional question for future investigation :** What happens if you include third order in perturbation theory or more $\hbar\omega$ excitations? How are the results affected if you use your model space from part (a)?

Supplementary information

Please create a model space with the following orbits

Proton	Neutron
$0d_{5/2}$	
$0d_{3/2}$	$0d_{3/2}$
$1s_{1/2}$	$1s_{1/2}$
	$0f_{7/2}$
	$1p_{3/2}$

The format of model spaces in proton-neutron formalism is found in Lecture III
or copy and modify an existing *.pn.sp from the sps folder