TALENT Course 6
Theory for exploring nuclear reaction experiments
NuShellX shell model code tutorial

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1 Introduction

This tutorial covers the use of the shell model code NuShellx@MSU. NuShellx was written primarily by Bill Rae. NuShellx@MSU contains the core NuShellx codes and additional wrapper input/output codes written by Alex Brown. The first thing to do is to connect to the talent server. This can be done from the local desktop machines by double clicking on the `Remmina` icon on the desktop. On laptops, if you have `rdesktop` installed you can connect using:

```
rdesktop -u USER -g 1024x800 172.16.39.38
```

If you do not have `rdesktop` installed the same command can be run after connecting to the talent server via ssh.

This tutorial assumes that NuShellx has been correctly set up, and is installed in the directory `TalentShare\aaa\` on drive `C:\`. The NuShellx command prompt can be started by opening the shortcut in the folder `C:\TalentShare\aaa\`.

2 Tutorial Overview

The objective of the tutorial is to calculate levels and spectroscopic factors relevant to one-proton removing reactions from ^{26}Ne - for example, one-proton knockout or ^{26}Ne$(d,^3$He$)^{25}$F. The calculations proceed in three steps. First we must calculate the levels for the initial nucleus of ^{26}Ne. Next we must calculate the levels of ^{25}F - the final states. Lastly, we must calculate the overlap between the ground state of ^{26}Ne and all the excited states of ^{25}F.

1. Open the NushellX shortcut in the `C:\TalentShare\aaa\` folder.

2. The command prompt should have opened successfully, and you should be in the directory `C:\Users\`. If this is not the case, navigate to this directory.

3. All calculations should be kept within your own directory. First, cd into the directory named for your username. Then within this directory, create a subdirectory called nushellx (type mkdir nushellx, hit return). Then move into this directory (cd nushellx).

4. NuShellx consists of a number of executables that are run in a specific sequence to perform shell model calculations. The interface to NuShellx is provided by the shell program. Shell asks questions to define the desired calculations and then produces a batch file to perform the calculation.

3 Level Calculations

1. First make a directory to contain the calculations, e.g. `mkdir ne26`. Then move into this directory - you should be in `C:\Users\USERNAME\nushellx\ne26`.

2. We will first make a calculation for ^{26}Ne. Before we begin, type `lab` and hit return. This opens the file `C:\TalentShare\aaa\nushellx\sps\label.dat` that contains the list of model spaces and interactions available to NuShellX. Keep this file open.

3. First, make sure you're in the correct directory (!), then type `shell` to start.

4. The first question asked is the name of the batch file. Since we are making a calculation for ^{26}Ne, let us name our batch file `ne26`. Note that no extension (e.g. .bat) is required. Shell will produce a batch file name `ne26.bat` that we will need to run to perform the shell model calculation. It will also produce a file named `ne26.ans` that contains the answers to all questions asked. More on this later.

5. Shell then asks for an option. There are two options for calculation `lpe`, for calculating wave functions and levels, and `den` for calculating overlaps. All calculations will first require some levels calculations, so we begin here. Type `lpe` and hit return.

6. Shell then asks for the model space name. Here, we need to refer to label.dat. There are several model spaces that would apply to ^{26}Ne, but for the time being we use the simplest the sd-shell. Find the code for the sd-shell model space in `label.dat` and enter it (sd).

7. Shell then asks if restrictions are required. This would allow us to truncate the model space. For the present case we do not require any truncations, so enter n.

8. Shell then asks for the interaction name. Under the sd model space, several interactions are listed, including the popular usd, usda and usdb. Enter the code for usd (w) and hit return.

9. Shell then asks for the number of protons. This is simply the number of protons for ^{26}Ne (10). Note that previous codes (Oxbash) had asked for the number of valance nucleons, rather than the absolute number.

10. The number of valence protons (6) should then be returned. Shell then asks for the total number of valence nucleons (i.e. the mass number, 26)

11. Shell then asks for the minimum and maximum for the spins of the final states in ^{26}Ne. Here we will enter 0.0, 6.0. The delJ is optional. This defaults to 1.0, and can usually be ignored.

12. Finally, shell asks for the parity of the states to be calculated. Within the pure sd-shell model space, only positive parity states are present, so enter 0.

13. Shell then lists some of the output files that will be generated. In principle we can now perform another calculation using `lpe`, or calculate some overlaps using `den`. In the case of the former, we do not need to re-enter the model space and interaction details, since they are assumed to be the same. For now, type `st` (stop) to end the calculation.

14. Back at the command prompt, the calculation can now be run by typing `ne26.bat`. The calculation may take a few minutes - hopefully it will work, but if you get any error messages, ask for help.

4 Level Output

1. Output files for NuShellX have a particular naming convention. They consist of a series of 6 letters and numbers that identify the model space, the interaction, the numbers of valance protons and neutrons, the parity and the spin. See the help file or the last page of this document for more information (taken from the help file).

2. We now can look at some of the output files from NuShellX. A summary of the calculated levels can be found in the file `ne26w.lpt`. This is our batch file name, followed by the interaction code, followed by the `.lpt` file extension. Type `dir *.lpt` to find the level summary file. There will also be a summary of experimental levels, in our case named `ne026exp.lpt`, and plots of the experimental and theoretical levels in two eps files, `ne26w.eps` and `ne026exp.eps`. You can open these by typing `gsview si024exp.eps`.

3. Further details about the calculated levels can be found in the `.lpe` files. For each state, these give the average occupancies for each orbital, and the decomposition for different total angular momentum couplings of protons and neutrons. Take a look at `bw2a00.lpe` using `notepad bw2a00.lpe`.

4. This file contains the information about the 0^+ states in ^{26}Ne. In the file name, the first letter stands for the model space code (b=sd), the second for the interaction (w==usd), third for the number of valence protons (2), fourth for the number of valence nucleons (a=10), fifth for the parity (0=positive, 1=negative) and the sixth for twice the spin (0).

5. The file begins with a summery of the interaction and model space used. There are a list of partitions for protons and neutrons. A partition is just a particular combination of placing the available nucleons in the active valence orbitals. These are referred to later when looking at the decomposition of the wave functions. The first number is the partition index, and the following six list how many nucleons are in each orbit for each partition. The first three numbers are the proton sd-shell orbits, the last three are the neutron orbits. The ordering of orbits matches the interaction in this case, $0d_{3/2}$, $0d_{5/2}$ and $1s_{1/2}$. This information is also given right at the bottom of this file.

6. Next are the details for each individual state. For state number 1 the binding energy is given as -81.62506. Then for each of nucleons type A and B (one is protons, the other neutrons, as stated at the top of the file), the average number of nucleons in each orbit are given.

7. After this, a more complex decomposition of the state is given. The protons and neutron partitions are treated separately, and the wave function is decomposed into different sections of total angular momentum couplings A and B. For example, 81.35678% of the time the total angular momentum for both protons and neutrons is zero. Further down, the percentage of the wave function when both protons and neutrons are coupled to total angular momentum 2 is 16.04640%.

8. Move back to just below the line with 81.35678%. This fraction of the wave function is then decomposed into individual partitions. For example, 4.801% of the time, the protons (nucleons B) are in partition number 1 (with their angular momentum coupled to zero). Partition 1 for type B nucleons has two protons in $d_{3/2}$. Below this, the decomposition continues to the type A nucleons (neutrons). For example, of the full wave function 3.68% has the neutrons in partition 12 coupled to total angular momentum 0 and the protons in partition 1 coupled to angular momentum 0.

9. This decomposition continues for all couplings and partitions above a certain thresholds.

5 Modifying shell Inputs

1. If we made a mistake when giving answers to `shell`, we do not necessarily need to re-enter all the information again. The answers are saved in a file ending on `.ans`. This file can be edited and then read by shell by giving the full file name (e.g. `ne26.ans`) when prompted by a file name by shell.

2. We could, for example, run the same calculation again but using a different interaction. However, these calculations should always be done in a different directory.

6 Calculating overlaps

1. Suppose we wish to calculate the spectroscopic factors for proton knockout from ^{26}Ne. We have the levels for ^{26}Ne already - we only need the ground state. But we also need

levels calculations for the final nucleus ^{25}F. Run shell again and create a new batch and answer file to calculate the levels of ^{25}F from $1/2^+$ to $5/2^+$ with the USD interaction. Do this in the same directory as the ^{26}Ne calculations. Then run the batch file.

2. Type dir *.lpe to list the calculated levels. You should see three sets of files. Those beginning with bw1 are ^{25}F with USD, those starting with bw2 are ^{26}Ne with USD and those starting ba2 are ^{26}Ne with USD.

3. We first need to run shell to calculate the overlaps and generate one-body density files. Run shell and enter a file name for the batch job (e.g., `overlap`).

4. Choose option `den` for overlaps, then option 1 for spectroscopic factors. (Options 1 and 2 are for calculating one- and two-particle spectroscopic amplitudes respectively). Option t is for calculated transitions (e.g. $B(E\lambda)$ or $B(GT)$).

5. Enter the initial file name. This is the name of the level file for ^{25}F, without the file extension. Enter `bw1901`. From this shell deduces the models space (b), interaction (w), number of valance particles (1,9) and the parity (0), but we will be given the option in a moment to enter a range of J values to calculate over.

6. Next shell asks for the maximum number (of states) for each J. Enter -1; This will calculate the overlaps for all final states in ^{25}F.

7. Enter the relevant information for the final state. The file name is bw2a00. Enter 1 for the number of states - we only want the overlap with the ground state of ^{26}Ne.

8. Now we may enter the ranges of J. Enter 0.5,2.5 for the initial state (^{25}F), and 0.0,0.0 for the final state (^{26}Ne).

9. Enter n to not restrict the coupling operator, and enter st to end the batch file.

10. If you made any mistakes simply correct the answer file, overlap.ans, and rerun shell. Then run the batch file (`overlap.bat`).

11. Once the batch file has run, the results for the spectroscopic factors can be found in `.lsf` files. The file `ne26w.lsf` will contain all spectroscopic factors calculated. Compare your results for $5/2^+$ states to those presented in the morning. NuShellX spectroscopic factors already have the isospin Clebsch-Gordan coefficient included, but account for this they should agree with those presented.

7 Extension: re-run the calculations using the USDA interaction

By copying the `.ans` files you have already used into a new directory and modifying them, run the calculations again using the USDA interaction. Are there any differences in spectroscopic factors and levels?

8 Extension: ^{28}Mg and two-nucleon amplitudes

Here the idea is very similar to the above. In this case we want to study two-nucleon amplitudes. We first calculate levels for ^{28}Mg and ^{26}Ne, and then calculate the overlaps by specifying the initial and final wave function names. This time, we need to use option 2. The server may not be able to cope with these calculations, even for one person, so proceed with caution!

10.2 Names for the wavefunction and overlap files

The first part of the file name for wavefunctions has the six letter form **abxypj** where:

```
a - symbol for the model space found in label.dat
b - symbol  for the interaction found in label.dat
x - sympol for the number of valence protons
y - symbol for the number of valence nucleons
p - symbol for the parity (0 for + and 1 for -)
j - symbol for two times the spin from the list below
```

The first part of the names for overlaps has the nine letter form **ABXYPJ**$_x$**ypj** where **ABXYPJ** is the name of the initial state and **xypj** is part of the name of the final state.

If the model space and interaction name do not exist in label.dat they will be assigned the names **x** and **y**, respectively.

The symbols for J, T and N correspond to the following numbers

```
0 - 0     k - 20    f - 40    0 - 60    h - 80    f - 100   0 - 120
1 - 1     l - 21    g - 41    1 - 61    l - 81    g - 101   1 - 121
2 - 2     m - 22    h - 42    2 - 62    m - 82    h - 102   2 - 122
3 - 3     n - 23    i - 43    3 - 63    n - 83    i - 103   3 - 123
4 - 4     o - 24    j - 44    4 - 64    o - 84    j - 104   4 - 124
5 - 5     p - 25    k - 45    5 - 65    p - 85    k - 105   5 - 125
6 - 6     q - 26    l - 46    6 - 66    q - 86    l - 106   6 - 126
7 - 7     r - 27    m - 47    7 - 67    r - 87    m - 107   7 - 127
8 - 8     s - 28    n - 48    8 - 68    s - 88    n - 108   8 - 128
9 - 9     t - 29    o - 49    9 - 69    t - 89    o - 109   9 - 129
a - 10    u - 30    p - 50    a - 70    u - 90    p - 110   a - 130
b - 11    v - 31    q - 51    b - 71    v - 91    q - 111
c - 12    w - 32    r - 52    c - 72    w - 92    r - 112
d - 13    x - 33    s - 53    d - 73    x - 93    s - 113
e - 14    y - 34    t - 54    e - 74    y - 94    t - 114
f - 15    a - 35    u - 55    f - 75    a - 95    u - 115
g - 16    b - 36    v - 56    g - 76    b - 96    v - 116
h - 17    c - 37    w - 57    h - 77    c - 97    w - 117
i - 18    d - 38    x - 58    i - 78    d - 98    x - 118
j - 19    e - 39    y - 59    j - 79    e - 99    y - 119
```