Tutorial on shell model calculations and the production of nuclear Hamiltonians

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Tutorial of the *Espace de Structure Nucléaire Théorique*

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I. PROBLEM SET 1

For this set of problems, please use the sd.sp model space file with the usdb.int interaction file. Both are found in the sps folder and described in label.dat for reference, but NUSHELLX will find them for you and put them in your working directory. The model space and interaction are in the 't' formalism discussed in the lectures ; the corresponding examples in 'pn' formalism are sdpn.sp and usdbpn.int. Utilize default values as the answers to 'shell' prompts if unspecified below.

1. $A = 24$ nuclei
   (a) Calculate the level schemes (lpe option in shell) up to $J = 4$ for ^{24}Mg, ^{24}Ne, and ^{24}Si. You only need to execute shell once if you choose the lpe option three separate times. For ^{24}Mg, produce 20 eigenvalues for each J value by typing 'lpe,20' inside the 'shell' executable. The three calculations combined should take approximately 5 minutes to run.
   (b) Compare the theoretical results to the available experimental data (plotted in *24b.eps files). Compare the results to the approximate rms deviation of 126 keV for the USDB interaction. On the left side of ne24b.eps, the black dots correspond to observed states with unassigned J^π values from the ENSDF database. What J^π value would you predict for the state at 4.886 MeV ? What about the two states at 5.636 MeV and 5.653 MeV ?[1] The last ENSDF compilation occurred in 2003. Hoffman et al. [Phys. Rev. C **68**, 034304 (2003)] have since assigned J^π values for these three experimental states.
   (c) What do you observe about the symmetry of the USDB interaction ? At what excitation energy does the first $T = 2$ state occur in ^{24}Mg (the *.lpt files tabulate all calculated levels) ?
2. Mass of a nucleus
   (a) Calculate the ground state energy of ^{30}Al. Include the Coulomb correction for USDB[2] (21.48 MeV for $Z = 13$). Compare to the experimental mass excess of -15872(14) keV by neglecting the electron binding energy BE_e. How could the theoretical value be improved ? Beyond the masses below, another value is necessary and can be obtained from the 'toi' executable in NUSHELLX. See supplementary information if you need formulas.

$$\begin{aligned} m_u &= 931.494\text{MeV}/c^2 && \text{atomic mass unit} \\ m_p &= 938.272\text{MeV}/c^2 && \text{proton mass} \\ m_n &= 939.565\text{MeV}/c^2 && \text{neutron mass} \\ m_e &= 0.511\text{MeV}/c^2 && \text{electron mass} \end{aligned}$$

3. Spectroscopic factors
   (a) The reaction ^{34}S(d,^{3}He)^{33}P has been used to study the properties of ^{33}P by Thorn et al. [Phys. Rev. C **30**, 1442 (1984)] and Khan et al. [Nucl. Phys. A **481**, 253 (1988)]. Both have extracted "experimental" spectroscopic factors. In the independent particle model, what are the $C^2S^\pm$ values for ^{34}S ? Recall that NUSHELLX employs the sum rule (for 0^+ states in a reduced model space)

$$(2j+1) = \sum_i C^2S_i^- + (2j+1)C^2S_i^+$$

1. It is difficult to distinguish these two points on the scale of the plot, but there are two unassigned states.
2. B.A. Brown and W.A. Richter, Phys. Rev. C **74**, 034315 (2006)

(b) Calculate the ground state of ^{34}S and all states in ^{33}P for which spectroscopic factors can be found. The wavefunction of the ground state of ^{34}S is given in bb8i00.lp. The partitions are listed near the top of the file, with ordering consistent with the model space in sd.sp. What percentage of the total wavefunction is in the expected single particle configuration from the independent particle model, accounting for both protons and neutrons? What is the next most likely configuration of protons? What percentage of the wavefunction comes from $J_p = J_n = 0$?

(c) Calculate spectroscopic factors with the den option in shell. Note that the initial wavefunction must be the lighter ^{33}P nucleus called bb7h01, for instance. Perform the calculation with only the ground state of ^{34}S but all calculated ^{33}P states by choosing max number -1 for inital and 1 for final states.

(d) Compare the output in the *b.lsf file to the experimental data below (all from Khan et al. except last column). The variation between experimental spectroscopic factors is significant. Which experiment is reasonably consistent with the calculation?

E_x (MeV)	J	C^2S	C^2S_{Thorn}
0	$\frac{1}{2}$	1.36	2.2
1.435	$\frac{3}{2}$	0.73	0.37
1.843	$\frac{5}{2}$	1.26	1.26
3.250	$\frac{3}{2}$	0.15	0.06
3.480	$\frac{5}{2}$	0.36	0.19
4.050	$\frac{5}{2}$	1.48	0.46
5.050	$\frac{5}{2}$	1.91	0.34

4. Electromagnetic transitions

(a) Calculate the lowest 0^+ and 2^+ states for all even-even neon isotopes in the model space.

(b) Use the den option in shell to calculate the $B(E2)$ transitions from the first excited state to the ground state. NUSHELLX gives the output in this direction in *.deo files, but note that the transition $B(E2; 0^+ \to 2^+)$ would be five times larger.[3]

(c) Compare to the experimental data below.[4] Is there a correlation between $E(2^+)$ and $B(E2)$? Which isotopes result in the largest disagreement between theory and experiment? What is the cause?

^{A}Ne	$E(2^+)$ (MeV)	$B(E2)(e^2\text{fm}^4)$
18	1.89	49.6
20	1.63	65.5
22	1.28	45.8
24	1.98	28.0
26	2.02	50.0
28	1.30	26.0
30	0.79	92.0

Supplementary information

$$m(Z,N) = Zm_p + Nm_n - BE(Z,N)/c^2$$
$$m_{\text{atom}} = m(Z,N) + Zm_e - BE_e$$
$$m_{\text{atom}} = Am_\mu + \Delta/c^2$$

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3. Regardless of your selection of input and final state in 'den', NUSHELLX always determines $B(E2)$ from the higher energy state to the lower energy state. To get the value for the "up" direction, for instance as they are typically given in Coulomb excitation experiments, you must account for the $\frac{2J_i+1}{2J_f+1}$ factor. You can have NUSHELLX do this by editing the x.den file, changing the order of the J_i, J_f, T_i, T_f line below e2,10, and then running dens < x.den <enter> gamma x <enter>

4. A recent experiment by Gibelin et al. [Phys. Rev. C **75**, 057306 (2007)] measured a new value of $B(E2) = 28.2e^2\text{fm}^4$ in ^{26}Ne, suggesting evidence for a subshell closure at $N = 16$.