Tutorial on shell model calculations and the production of nuclear Hamiltonians

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Tutorial of the Espace de Structure Nucléaire Théorique

13 May - 17 May 2013

CEA/SPhN, Orme des Merisiers, build. 703, room 135, F-91191 Gif-sur-Yvette Cedex

I. PROBLEM SET 5

- 1. The Monopole part of the interaction : Microscopic vs. Phenomenological
 - (a) In the sps folder, find the usdb interaction. Calculate the T=1 monopoles (d5d5, d5d3, d5s1, d3d3, d3s1, s1s1) according to the formula given in lectures :

$$V_{ab}^{T=1} = \frac{\sum_{J} (2J+1) V_{abab}^{JT}}{\sum_{J} (2J+1)}$$
(1)

Compare with the figure of USD monopoles.

- (b) Now calculate the *sd*-shell matrix elements for a low-momentum interaction starting from any NN potential with momentum-space cutoff $\Lambda = 2.0 \,\text{fm}^{-1}$. Go to 2nd-order in MBPT choosing a reasonable size HO basis for intermediate states ($l_{max} = 6$ or hw=4 in the input file).
- (c) Calculate the T=1 monopoles for this interaction that you've created. How do these monopoles compare to the phenomenological values? What type of strength is needed to bring the microscopic picture closer to phenomenology (*i.e.*, data)?
- 2. Density Dependent 3N Interaction
 - (a) Now we're going to create a *density-dependent* 3N interaction. This is in general very complicated, but we can rather easily consider only the 3N contact term. So we need to go into the code and change it first to *only* calculate a contact interaction. Go to the "hamre" folder and find the routine renorm-potentials.f. Save a backup copy (renorm-potentials-save.f) first !!!
 - (b) This file contains the code to calculate all NN interactions, so it's very large. Open this file and search for "n3lo" (line 11495). For all searches below, make sure you are searching down through the file not up, as there is a routine above which has similar statements, and we don't want to change that one.
 - (c) From here search for "8000 continue". Immediately after this add a line : "goto 8030". This will skip one-pion exchange.
 - (d) Next search for "8105". You should see the line "8105 v(iv)=v(iv)+vj(iv,il)" Change this to 8105 v(iv)=v(iv)+vj(iv,il)"
 - (e) Right below this, you should see "do 8155 il=iman9,imen24". Comment this out and add replace it with "do 8155 il=iman9+6,iman9+6"
 - (f) Below this change "8205 vv0(iv)=vv0(iv)+vj(iv,il)" to "8205 vv0(iv)=vv0(iv)!+vj(iv,il)"
 - (g) Next one : change "8215 vv2(iv)=vv2(iv)+vj(iv,il)" to "8215 vv2(iv)=vv2(iv)!+vj(iv,il)"
 - (h) Ok, last one : change "8225 vv4(iv) = vv4(iv) + vj(iv,il)" to "8225 vv4(iv) = vv4(iv) + vj(iv,il)"
 - (i) Now the code will only calculate one contact interaction, and we just have to make it the one we want. So finally we're going to change the code to calculate the density-dependent interaction from Holt, Kaiser, Weise Phys. Rev. C 81, 024002 (2010).

$$V_{NN}^{med,6} = -\frac{3M_N c_E \rho}{8\pi f_\pi^4 \Lambda_\chi} \tag{2}$$

So search for "3000" until you find the line "3000 c(mm,im)=3.d0/(16.d0*pi2*fpi4)". Comment this out and add for now the line "3000 c(mm,im)=3.0*0.625/2.0*0.16*(197.327/939.0)**3 /(92.4/939.0)**4/(700.0/939.0)". Be sure to put in a line break, otherwise it will extend past column 72, which for tran 77 doesn't like. This is the formula above, where everything is in units of MeV/ M_N . And I've used standard values for $\rho = 0.16$ and $c_e = -0.625$. Remember this, as well be changing these (and only these) later.

- (j) Last thing now is to search for "3005 aa(i)=aa(i)*c5*ell(i)*brak" and change it to "3005 aa(i)=aa(i)*c5!*ell(i)*brak". We're done! Just save and exit (we'll compile later).
- 3. Momentum space matrix elements
 - (a) Now that we can calculate the effects of a 3N contact interaction in our NN format, we want to make sure we've done everything correctly. So let's write out the momentum space matrix elements for this. The code for some reason doesn't do this automatically, but we can make it do so rather simply. Open the file renorm-vlowk.f90 (again, save a backup first !!!).
 - (b) Now search for "CALL vlowk_mtx(ncoup,vzz,heff,i)". Right after the ENDIF immediately below it, add the following lines :

DO ii = 1,n_k1 DO jj = 1,n_k1 if (ncoup == 1)then write(6,'(2I4,E14.6)')ii,jj,real(heff(ii,jj))*(197.327)**3*3.7851E-002 elseif (ncoup == 2)then write (6,'(2I4,4E14.6)')ii,jj, & real(heff(ii+n_k1,jj)), & real(heff(ii+n_k1,jj)), & real(heff(ii,jj+n_k1)), & real(heff(ii+n_k1,jj+n_k1)) endif ENDDO ENDDO

Just define the integer variables "ii" and "jj" above, exit and compile.

- (c) Run the code and look at the momentum space matrix elements printed out in the file *.reout. The momentum space mesh is given at the top of the file right after the line "points for ho oscillator basis". Locate (they will be several screens down) and make sense of the matrix elements you've written out for each partial wave. Do they look like you'd expect? In particular compare with Figure 5 in the above article.
- 4. Monopoles of 3N contact
 - (a) Finally take the interaction you've created and calculate the monopoles. How do they compare with what we would like?
 - (b) Choose several combinations of different values for c_E (from -1.0 to 1.0) and ρ and see if you can improve this.
 - (c) When you're done be sure to copy your "save" backups back into renorm-potentials.f so you don't end up using this 3N contact for the rest of your calculations!