From: Tom Rescigno <kingkohn@pacbell.net>
Subject: notes and input files for the mesa and scattering codes
Date: March 17, 2013 10:49:54 PM CDT
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1 Attachment, 8 KB

Bob,
I'm attaching a set of input files for the CO2 case we talked about. In general, here's how it goes.
First, you determine the total number of configurations (NCSFS) - P-space terms plus all (uncontracted) Q-space terms - in the usual fashion. The set of uncontracted Q-space terms are going to be replaced by a smaller number of contractions, in linear combinations based on the P-space target vectors, when constructing the optical potential and the full scattering wave function. To this set of Q-space vectors, we can add an additional vector which can be an eigenfunction of the full set of Q-space terms. There are cases where you'd want to do this. For example, in electron + F2 scattering, F2^- is bound in sigma-u symmetry. If you contract Q-space and don't allow it to contain the full F2^- vector, then you might get a phoney low-energy shape resonance instead of a bound negative ion. I don't think you need this option in photoionization, since the initial state is still going to be determined by finding an eigenvector of the full Q-space, not the contracted space, in the last MESA run, but I included the option in any case.

So here's the sequence.

1. You do a setup run (use mesa.inp.set)

2. You determine a Q-space eigenvector which is put on the mesa.kohn file (use mesa.inp.addqci). You specify which root you want on the kohn line with ciqroot=#. Note that only Q-space configurations are specified in the DRT input. I had to modify m902 to open the mesa.kohn file when ciqroot is specified on the kohn line.

3. You determine the Q-space contraction vectors with m928 (use mesa.inp.contract). The DRTs are set up as in a phot run: P-space represented with dummy orbitals plus all the q-space configurations. The kohn line has a bunch of new terms. core=5 denotes that 5 orbitals are doubly occupied in all CSFs. addqci specifies that the Q-space eigenvector, computed in the previous run, will be added to the contracted Q-space vectors. reorderqci specifies that the added vector will be shifted to the beginning of the Q-space vector list and normqci specifies that the Q-space vectors will be renormalized after the additional vector is added. smallsq, smallcq and smlqci are cutoff thresholds used in detemining how many Q-space vectors to keep. smallcq is used first. After all possible Q-space vectors are computed (number of target states times number of valence (nsmall-core) orbitals), those with norms less than smallcq are tossed. Then the vectors are successively orthonormalized, tossing vectors at each step with norms less than smallsq. Finally, the extra (addqci) vector is added and the orthonormalization procedure is repeated with smlqci. Make sure print=m928 is in the route to see what is happening.

4. You then do the optical potential run (use mesa.inp.opt). Note that the kohn line contains "contractq", specifying that Q-space is being contracted. hqq and freeze must be used. I modified m935 to handle the changes.

5. The scattering codes, up to csolve, are run as before. The input to csolve has "contractq" on line 3. After the linear equations are solved to get Q\Psi in the contracted space, the solution is re-expanded into the original uncontracted representation.

6. All the remaining steps (cdipc, final MESA run with mesa.inp.phot and cphot) are run without modification.

If you want to generate the mesa.chk file I've used, run MESA with mesa.inp.ci, followed with a run using mesa.inp.getno

Let me know if I can help with anything,
Tom

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inputs.zip (8 KB)