X.J. SAMQUA: RESONANCE QUANTUM NUMBERS

The code SAMQUA can serve as an aide to generating the correct (and complete) set of resonance spin quantum numbers for any given set of incident and exit channels. The original version of this program was quite limited, assuming a neutron incident on a single nuclide, and including only elastic channels. In 2003 Bouland and Babut of Cadarache, in collaboration with the SAMMY author, developed a more general version of this code [OB03]. This version of SAMQUA treats the general case of elastic, inelastic, reaction, and fission channels, including charged particles as needed.

Two distinct modes of input are available for SAMQUA. The first (the Cadarache input mode) uses free-format values interspersed with descriptive information, and is described in detail in the SAMQUA documentation [OB03]. The second (the Particle-Pair mode) uses essentially the particle-pair information from SAMMY's card set 4 of Table VI.A.1. In both cases, the output consists of portions of the SAMMY INPut file: Output file "quantum2.dat" contains card sets 4 and 10.2, as well as the necessary commands (to be included in card set 3 of the INPut file) for use of those input options. Output file "quanpar.dat" may be used (perhaps with modifications) for card set 7 (radius parameters) and card set 10 (isotopic abundances) of the SAMMY PARameter file. Another output file, "table.dat", gives the spin group information in tabular form.

One additional output file, "quantum.dat", contains card set 10.1 (for SAMMY's INPut file) plus command lines. However, use of this option in SAMMY runs is discouraged as the format is crowded, awkward, and non-intuitive and will eventually be disallowed. SAMMY users are encouraged to convert to card set 10.2 (as given in quantum2.dat of SAMQUA output).

Subsequent to publication of the SAMQUA manual [OB03], the code has again been upgraded [OB04] with options to provide additional information to the user, and to reorganize the output. For each run, another output file ("quantum3.dat") is created. This file contains the same information as quantum2.dat, with extra lines following each channel descriptor in card set 10.2; the extra lines give penetrability and hard-sphere cross section at specified energies. (The hard-sphere cross section is that cross section that would be calculated if there were no resonances.) By default these energies are 1.0 eV, 500 keV, and 1 MeV, but (for the particle-pair input mode) there are other options:

(1) The user can specify values Emin and Emax, and SAMQUA will calculate penetrabilities and cross sections at Emin, (Emin+Emax)/2, and Emax.
(2) A list of energies can be given in a separate file; this can be a SAMMY PARameter file or a simple list of energies.

Because the calculation of penetrabilities and cross sections requires knowledge of radii, and the radii used in an evaluation may differ from SAMQUA's default values, the user may also provide radii values.