Description of utility-programs for scattering problem in the DBSR complex (folder SCT\_JJ)

SEC\_DCS\_JJ

|  |  |
| --- | --- |
| Description: | provides differential and angle-integrated (ordinary and momentum transfer) cross sections for given transition |
| Input files: | zarm.tma (or zarm.tmb, tmat.done), target\_jj |
| Output files: | dcs\_ii\_ff, mt\_ii\_ff |
| Call as: | sec\_dif\_JJ itr1=ii itr2=jj i16=-1|0|. ifano=0|1 ek1=... ek2=... or ekk=… Glow=... Ghigh=... Gstep=... dcs=0|1 tdone=0|1 JJ\_extend=… |

All arguments are optional.

|  |  |
| --- | --- |
| itr1 [1] | index of initial state (default - 1) |
| itr2 [1] | index of final state (default - 1) |
| i16 [16] | i16 - controls the output units:  = 0 - sigma in a.u.  > 0 - sigma in 10-i16 cm2 |
| ifano [0] | = 0 - Condon-Shortly phase convention, default  = 1 - Fano phase convention |
| ek1 [0] | if > 0, restriction on minimum electrovn energy (in Ry) |
| ek2 [0] | if > 0, restriction on maximum electron energy (in Ry) |
| ekk [0] | if > 0, exact electron energy (ek1=ek2=ekk) (output in tmat.done\_inp) |
| Glow [0] | lowest scattering angle |
| Ghigh [180] | highest scattering angle |
| Gstep [1] | step fort scattering angle |
| dcs [1] | if = 0, skip the calculations of differential cross sections |
| tdone [0] | if =1, redirect input from zarm.tma to tmat.done file |
| JJ\_extend [0] | if > 0, extrapolate T-matrix elements to JJ\_extend value  (input tmat.done\_inp -> output tmat.done\_out) |

The utility SEC\_DIF\_JJ first check zarm.tma (zarm.tmb) file and create tmat.done file with T-matrix elements, specific for the given transition. The tmat.done file has the same format as in program MJK (Grum-Grzhimailo 2003). If ekk parameter is not equal 0, the program additionally analyzes the T-matrix elements for the given energy and prepares them for extrapolation to higher J-values. To do it, the program first divided all matrix elements on subsets with the same changes of involved l- and j-values. The values in subsets are supposed to reduce as in geometric series. The corresponding coefficients are found as ratio of two highest values in the series, T(n)/T(n-1). This information is recorded in the tmat.done\_inp file and the program stops. The user may check the extrapolation coefficients (in the end of the tmat.done\_inp file) and rerun the program with JJ\_extend parameter. The program with extrapolate the T-matric coefficients with 2J values up two JJ\_extend. The resulting T-matrix elements are recorded in tmat.done\_out file and program stops. The user may check extrapolated data and copy this file to tmat.done. Then, in order to get differential cross sections, he can use SEC\_DIF\_JJ with tdone=1 option, or any other program, which employ the tmat.done input. Note that for high J-values of J (> 50), the SEC\_DIF\_JJ program may take too much time due to big number of Aλ coefficients (see below). In this case, it is advised to use SEC\_DIF\_JJ\_ampl program (described below), which is much faster.

Related theory:

JJ –coupling (neutral case)







;  - Fano factor, used only for Fano phase convention



Angle-integrated and momentum-transfer cross section can be express as:



JJ –coupling (Coulomb case)

DCS can be expressed as pure Coulomb scattering, interference term and potential term (first two only for elastic scattering, when initial state, *i*, equal final, *f* ).





 (should be checked)



SEC\_DCS\_JJ\_AMPL

|  |  |
| --- | --- |
| Description: | provides differential and angle-integrated (ordinary and momentum transfer) cross sections for given transition |
| Input files: | zarm.tma (or zarm.tmb, tmat.done), target\_jj |
| Output files: | dcs\_ii\_ff, mt\_ii\_ff |
| Call as: | sec\_dif\_JJ\_ampl itr1=ii itr2=jj i16=-1|0|. ifano=0|1 ek1=... ek2=... or ekk=… Glow=... Ghigh=... Gstep=... dcs=0|1 tdone=0|1 JJ\_extend=… |

The utility SEC\_DIF\_JJ\_AMPL used the direct calculations of scattering amplitude instead of analytical approach implemented in SEC\_DIF\_JJ. It has the same input argument and the same file structure. The SEC\_DIF\_JJ\_AMPL turned out to be much faster then SEC\_DIF\_JJ, especially for big T-matrix sets with high maximum J-values (50 and more).

Related theory:



(relative phase between the Coulomb and potential part (±*i*) is different in different publications)







Considering φ=0, we may rewrite expression as



(  - is given by program ALEGFM)



So, we may use direct calculation of scattering amplitude for different M’s and them sum their modules.

Angle-integrated cross sections (if needed) are then obtain direct integration of *dσ* by angles.

 