**SEC\_TOP\_CBE**

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| Description: | top-up procedure for the cross sections (CBE method for dipole transitions and geometric series for others) |
| Input files: | zarm.omb\_par, target |
| Output files: | zarm.omb\_top, zarm.omb (without top-up), sec\_top\_omb.log, sec\_top\_coef\_fail |
| Call as: | sec\_top\_CBE [par=.. top=.. jtr1=.. jtr2=.. ek1=... ek2=... tail=.. x=..] |

All arguments are optional.

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| par [zarm.omb.par] | file with input partial collision strengths |
| top [zarm.omb\_top] | file with output top-up collision strengths |
| ek1 [0] | if > 0, restriction on minimum electrovn energy (in Ry) |
| ek2 [0] | if > 0, restriction on maximum electron energy (in Ry) |
| tail [0.001] | tolerance for top-up procedure |
| x [0.2] | tolerance for geometric series coefficient (x-1), if smaller -> extrapolation |
| jtr1, jtr2 [0,0] | debug parameters: if ≠ 0, considered only one transition jtr1-> jtr2, with more information |

method [1] if =2, the CBE approximation is used for dipole transitions

Coulomb-Bethe approximation and partial-wave summation

In the Coulomb-Bethe (CBE) approximation, the incident electron is supposed not to penetrate the target at all. Therefore, one can neglect the short-range interaction and replace the whole electrostatic-interaction (radial part) by its asymptotic form which is correct at . Then

(1)

Let us restrict our consideration to the case of the dipole transitions with . In this case the integration over the angular variables for the collision strength can be carried out analytically (Burke and Seaton 1986), and for the partial collision strength we obtain the following expression

(2)

where

(3)

is the usual definition of the line strength for radiative transitions.

The Coulomb function has the saddle point at

(4)

and at the Coulomb function is very small, i.e. the incident electron almost does not penetrate this region. Therefore CBE is correct only for and for which is much larger than the mean radii and of the target states. From these considerations one can obtain the following condition of CBE validity

(5)

This condition is fulfilled only for very large and . However, since in the case of optically allowed transitions the sum over the partial cross sections converges very slowly, the use of the CBE approximation is very convenient, especially, for the evaluation of high-L contributions at high energies. Moreover, in this approach not only the analytical expressions for the evaluation of the partial waves can be obtained, but the analytical summation of all these contributions can be carried out as well. Let us introduce the following notation

(6)

Burgess et al (1970) have obtained analytical formulae for in the case of the dipole transitions. Their programing implementation ig given in set of routines incorporated in the STGF program (see fdip\_stgf.f in BSR/UTILS/SCT\_LS folder).

For the evaluation of the higher partial contributions it is necessary to evaluate the sums of Burgess (1974), based on the recurrent relations between Coulomb integrals (6), obtained the following relations:

 (7)

 (8)

Note that here the linear momentum *k* is replaced to the reduced one,  *κ → k/z*, where *z* is the ion charges. It is not clear how to use these relations for neutral case. In this case we can use the other relation:

 (9)

where *k* is the normal linear momentum. In terms of partial collision strengths, Buress & Sheorey (1974)

 (10)

Choosing of λ: 

Therefore, the sum over momenta up to infinity can be reconstructed on the basis of last two calculated partial collision strength. However, due to numerical instability for high *l*-values, it should be used with precautions. We use formula (10) with numerical partial collision strengths (after stgf or farm calculation) in the first sum, and the CBE values in the second term. It requires additionally determine the one-electron values based on the partial wave  values after R-matrix calculations, however, it can be applied in different coupling schemes (LS. JK, JJ).

The generalization of method to the case of the quadrupole transitions is discussed in Chidichimo and Haig (1989) and Chidichimo (1988).