SEC_TOP_CBE

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.

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 $r_1^{\lambda}/r_2^{\lambda+1}$ which is correct at $r_2 > r_1$. Then

$$K_{if,\lambda}^{CBe} = \int_0^{\infty} F_{l_i}(r_2) r_2^{\lambda-1} F_{l_f}(r_2) dr_2 \int_0^{\infty} P_{l_0}(r_1) r_1^{\lambda+1} P_{l_1}(r_1) dr_1 \qquad (1)$$

Let us restrict our consideration to the case of the dipole transitions with $\lambda = 1$. 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

$$\Omega(l_i, l_f) = \Omega(\Gamma_i S_i L_i l_i, \Gamma_f S_f L_f l_f) = \frac{16}{3} S(\Gamma_i S_i L_i, \Gamma_f S_f L_f) l_> \left| \int F_{k_i l_i} r^{-2} F_{k_f l_f} dr \right|^2 \qquad (2)$$

where

$$S(\Gamma_i S_i L_i, \Gamma_f S_f L_f) = \sum_{M_s, M_L, \mu} \left| \left(\Gamma_i S_i L_i M_{S_i} M_{L_i} \left| \sum_{n=1}^{N} C_{1\mu}(\hat{r}_n) r_n \right| \Gamma_f S_f L_f M_{S_f} M_{L_f} \right) \right|^2 \qquad (3)$$

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

The Coulomb function has the saddle point at

$$r_0 = \{[z^2 + k^2 l(l+1)]^{1/2} - z\}/k^2 \tag{4}$$

and at $r \ll x_0$ the Coulomb function is very small, i.e. the incident electron almost does not penetrate this region. Therefore CBE is correct only for l_i and l_f for which r_0 is much larger than the mean radii r_i and r_f of the target states. From these considerations one can obtain the following condition of CBE validity

$$l > \left(k^2\overline{r}^2 + 2z\overline{r} + 1/4\right)^{1/2} - 1/2 \tag{5}$$

This condition is fulfilled only for very large l_i and l_f . 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

$$I\left(k_i l_i, k_f l_f; \lambda\right) = \int_0^\infty F_{kl_i}(r) r^{-\lambda-1} F_{k_f l_f}(r) dr \tag{6}$$

Burgess et al (1970) have obtained analytical formulae for $I\left(k_i, k_j, \lambda\right)$ 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 $\Omega\left(l_i, l_f\right)$. Burgess (1974), based on the recurrent relations between Coulomb integrals (6), obtained the following relations:

$$\begin{aligned} S_\lambda &= \sum_{l=\lambda}^{\infty} l(I^2(k_i\lambda, k_f\lambda-1;1) + I^2(k_i\lambda, k_f\lambda-1;1) \;\propto \sum_{l=\lambda+1}^{\infty} (\Omega(l, l-1) + \Omega(l-1, l) \\ &= [(1+\lambda^2 k_i^2) I^2(k_i\lambda, k_f\lambda-1;1) - (1+\lambda^2 k_f^2) I^2(k_i\lambda-1, k_f\lambda)] / [\lambda^2(k_i^2 - k_f^2)] \end{aligned} \tag{7}$$

$$\begin{aligned} S_{\lambda+1} &= \sum_{l=\lambda}^{\infty} l(I^2(k_i\lambda, k_f\lambda-1;1) + I^2(k_i\lambda, k_f\lambda-1;1) \propto \sum_{l=\lambda+1}^{\infty} (\Omega(l, l-1) + \Omega(l-1, l) = \\ &= [(1+\lambda^2 k_f^2) I^2(k_i\lambda, k_f\lambda-1;1) - (1+\lambda^2 k_i^2) I^2(k_i\lambda-1, k_f\lambda)] / [\lambda^2(k_i^2 - k_f^2)] \end{aligned} \tag{8}$$

Note that here the linear momentum *k* is replaced to the reduced one, $\kappa \longrightarrow k/z$, 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:

$$\sum_{l=\lambda}^{\infty} \sum_{l'=l\pm1} l_> I^2(\kappa_i l, \kappa_f l';1) = [I^2(\kappa_i\lambda, \kappa_f\lambda-1;1) - I^2(\kappa_i\lambda-1, \kappa_f\lambda)] \frac{z^2 + k_i^2\lambda^2}{[\lambda^2(k_i^2 - k_f^2)]} \tag{9}$$

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

$$\Omega = \sum_{l=0}^{\lambda} \sum_{l'=l\pm1} \Omega(l,l') \; + \; [\Omega(\lambda,\lambda+1) - \Omega(\lambda+1,\lambda)] \frac{z^2/(\lambda+1) + k_i^2}{(k_i^2 - k_f^2)} \qquad (10)$$

Choosing of λ: $\lambda = \min(J_{\max}^{partial} - J_1^{target} - 1/2, J_{\max}^{partial} - J_2^{target} - 1/2) - 1$

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 $\Omega(l,l')$ values based on the partial wave $\Omega(l,l',\pi LS)$ 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).