Radiative Gaunt factors

Anca Ruxandra Diana Chelmus and Viorica Stancalie

National Institute forLaser, Plasma and Radiation Physics, LaserDept., P.O.Box MG-36, Bucharest, Romania

The radiative Gaunt factors are calculated on the basis of quantum mechanical definition and pseudo-state/ R-matrix numerical method for continuum states. A pair-coupling scheme is used to describe bound and continuum states of Be-like carbon, as an example. Fundamental atomic data and related plasma quantities are given for completeness.

1.Introduction

In the fitting of observed spectra for diagnostic analysis, it is generally the relative intensities of a set of connected spectrum lines which allow inference of underlying plasma parameters. It has been recognized that, for new approaches to spectroscopic measurement of enhanced diagnostic impact, earlier systematic large-scale production of atomic data should be done. The effective recombination and ionization rates and emissivities must be known (and at a finite electron density) for modeling and analysis the plasma. The light element ions, such as carbon ions, are radiators in the divertors of fusion plasma, albeit at higher electron densities and with strong influence of wall and recycling sources. Moving away from the divertor strike zones towards the confined plasmas, we progress through higher ionization stages up to the bare nuclei of carbon, nitrogen, oxygen along with protons and electrons. The emission, though, is complex, with a bremsstrahlung contribution along with spectrum lines which appears to be non-thermal.

Partially ionized ions of elements such as silver and palladium in the first long period, and tungsten and tantalum in the second long period, however, have two problems, an atomic structure which increasingly should be described in intermediate coupling and a consequent description of their emitted spectrum lines into very many separated levels from many transition arrays often associated with partially inner shells. The spectral emission may appear as a quasi-continuum. For the quasi-continuum, rather than individual lines, we can treat spectral intervals. Such spectral intervals can be those corresponding to particular spectrometer.

On the other hand, from the excited population models, synthetic spectra can be calculated and the significant point is the flexible separation of the spectra, which may be grass-like in their complexity at high resolution, into transition array envelopes at lower resolution which are characteristic of the emitter. The generalized collisional-radiative coefficients from the population codes provide the source terms for the ionization balance. To have a spatially non-equilibrium balance we need to express all these coefficients by using Gaunt factors.

This paper will summarized approximations used for evaluation of bound-bound, bound-free and free-free Gaunt factors. Application refers to Be-like C as an example.

2. Gaunt factors and derived atomic coefficients

The basic formulation for Gaunt factors is single configuration Russel-Saunders coupling. At the fine structure resolution level, the generalized Gaunt factors are written as [1]:

$g^{III}\left[\left(S_pL_p\right)\kappa lSLJ,\left(S_pL_p\right)\kappa' l' SL' J'\right]$ free-free

$g^{II}\left[\left(S_pL_p\right)\kappa lSLJ,\left(S_pL_p\right)\nu' l' SL' J'\right]$ free-bound

$g^{I}\left[\left(S_pL_p\right)\nu lSLJ,\left(S_pL_p\right)\nu' l' SL' J'\right]$ bound-bound

where S_pL_p denote the spin and orbital quantum numbers of the state γ (that is the parent state of the z +1 times ionized ion), ε, ε', κ, κ' are defined by $\varepsilon = \kappa^2 = E/z_1^2 I_H$, $\varepsilon' = \kappa'^2 = E'/z_1^2 I_H$ for free states ($z_1 = z + 1$), ν and ν' are the effective principal quantum numbers for the quantum shells *n* and *n'*, being defined by $\varepsilon = -1/\nu^2 = E/ z_1^2 I_H$, $\varepsilon' = -1/\nu'^2 = E'/ z_1^2 I_H$, for bound states . I_H =13.6 eV.

The most relevant groups of atomic coefficients for plasma modeling are the photon emission coefficients and the energy emission coefficients. The former enter the statistical balance equations (that is number of conservation) and the latter the energy balance equations. Maxwell averages of the

free-free and free-bound coefficients are also required for thermalised electron plasmas.

3. Calculations

Bound-bound, bound-free and free-free radial integrals are required for hydrogenic and non – hydrogenic ions. There are different approaches to calculate these integrals. Usually, semi-analytical methods based on the works by Burgess and Seaton [2], Peach [3] or Bates-Damgaard [4] are used to determine the asymptotic series expansions of the radial wave functions in the pure Coulomb regime. Moreover, closed analytical expression are available for the l summed Gaunt factors in the hydrogenic case [4]. Simple fittings to these ones have been given by Burgess and Summers [1].

In our work we used a pair-coupling, *jk* , scheme to calculate Gaunt factors. In a such description $J_i + l = K$ and $K \pm ½ = J$, where J_i is the total angular momentum of the target state, l is the orbital momentum of the added electron and ½ its spin. The Gaunt factor in *jk* coupling is written as follows:

$$g(k_i, k_{i'}) = \frac{2\sqrt{3}}{\pi} \sum_{l,l'} l \rangle \left| \int F_{k_i l_i} F_{k_{i'} l_{i'}} \frac{dr}{r^2} \right|^2 \quad \text{where } L_i + S_i = J_i, \; J_i + l_i = K \text{ and } K_s = J^T.$$

We have apply this formalism to calculate Gaunt factors for Be-like Carbon and to compare with those obtained by using hydrogenic approach. The pair coupling scheme requires to include as CIII symmetries : $^1S^e$, $^3P^e$, $^5D^e$ for $J=0^e$ and $^1P^0$, $^3S^0$, $^3P^0$, $^3D^0$, $^5P^0$, $^5D^0$, $^5F^0$ for $J=1^0$. After recoupling for $J=0^e$ and $J=1^0$, there are 28 and 72 channels, respectively. In our calculation, we used the effective quantum numbers obtained in the pseudo-state/R-matrix method, within the high optimization offered by close-coupling [5]. For $2p_{3/2}3p$ –ns series, bound-free Gaunt factor as function of photon energy is shown in Fig1, as an example.

It is well known that the Gaunt factor has a decreasing feature when photon energy is increased. By comparing our results with those calculated [1] in *LS* coupling at same energy range and using a hydrogenic approximation we can conclude on the following issues:

- the use of *jk* gives the proper description of many-electron atomic systems into the plasma;
- the alternative way of using the effective potential of Slater type, can be only regarded as an improved of the calculations;
- a new, more efficient, methods should be adopted to describe many electron systems into the plasma, which could replace the more sophisticated R-matrix code;
- to this aim, we have considered a recently developed perturbative approach for doubly-excited level positions [6];
- our results for effective quantum numbers are in very good agreement with those reported by K.Berrington in the Ref.5.

Table 1 shows part of these results:

Table 1

Effective quantum numbers relative to ^2S ionization threshold

state	this work	Ref.5.
2s3s ($^1S^0$)	2.64483	2.6649
4s	3.64148	3.6411
5s	4.52235	4.5649
10s	9.65381	9.6444
$2p_{1/2}5p(^3P^0)$	4.86043	4.8609
6p	5.85108	5.8614
7p	6.86591	6.8631

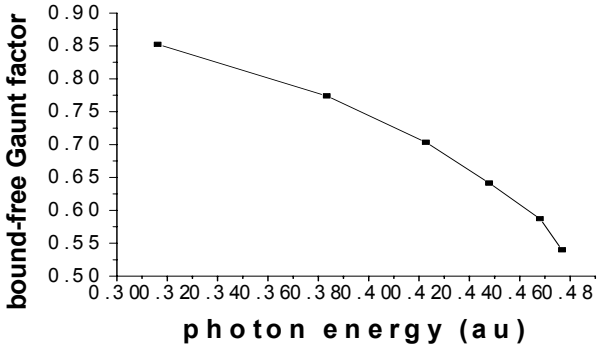

Figure 1. Free-bound Gaunt factor for $2p_{3/2}$ 3p-ns series in CIII

4. References

[1] A.Burgess, H.Summers, Mon.Not. R.astr.Soc. , **226**(1987)257

[2] A. Burgess, M.J.Seaton, Mon.Not. R.astr.Soc., **120,**(1960)121

[3] G. Peach Mon.Not. R.astr.Soc., **130**(1965)361

[4] D.R.Bates, A.Damgaard, Phil.Trans.R.Soc. A, **242**(1949) 101

[5] K. Berrington, J. Pelan, L.Quigley, Phys.Scr. **57** (1998)549

[6] M. Poirier, Phys.Rev. A**38**(1988)3484