EUROPEAN FUSION DEVELOPMENT AGREEMENT

EFDA-JET-CP(05)02-49

V. Stancalie and JET EFDA contributors

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New Method to Calculate the Gaunt Factor for the Refinement of Z_{eff} Evaluation in Fusion Plasmas

V. Stancalie[1] and JET EFDA contributors*

[1]Laser Department, National Institute for Laser, Plasma and Radiation Physics, P.O.Box MG-36,
Bucharest, 077125 ROMANIA, Association EURATOM/MEdC
** See annex of J. Pamela et al, "Overview of JET Results ",*
(Proc.20 th IAEA Fusion Energy Conference, Vilamoura, Portugal (2004).

Preprint of Paper to be submitted for publication in Proceedings of the
EPS Conference,
(Tarragona, Spain 27th June - 1st July 2005)

ABSTRACT

This work presents a perturbative approach for the evaluation of the effective oscillator strength averaged over continuum and Gaunt factors, for a particular case of complex atoms with two electrons outside closed shell. Based on the Coulomb formalism accounting for the general properties of the Coulomb Green's function, together with its available compact integral representations and discrete state expansions, results refer to Be-like C, Al and Ar, and Ba-like W ions, as an example. Such calculations are of interest as they represent accurate benchmark data for beam emission spectroscopy, Zeff analysis or complex atoms modeling in fusion plasma devices.

1. INTRODUCTION

Precise quantum –mechanical calculations of Gaunt factors exist only for hydrogenic species. Semi-analytical methods are used to determine the asymptotic series expansions of the radial wave functions in the pure Coulomb regime. Closed analytical expressions are available for the orbital quantum number, *l*, summed Gaunt factors, in the hydrogenic case. Simple fittings to these ones have been given by Burgess and Summers[1].

In the present work it is proposed an extension of the use of Rydberg states in the Coulomb formalism accounting for the general properties of the Coulomb Green's function, together with its available compact integral representations and discrete state expansions[2]. Coulomb bound-free matrix elements are computed numerically, avoiding the complex problem of uniform asymptotic expansion. Although, for dipole couplings the integrands can be, in principle, evaluated exactly performing the integration running onto continuous spectrum without severe technical difficulties. One way to get around this is to introduce the so-called '*averaged excitation energy'*. These representations are most useful as they provide elegant and efficient ways to compute values of high-order perturbative matrix elements in hydrogen, position of high Rydberg states, autoionisation probabilities, oscillator strength averaged over continuous spectrum, and consequently Gaunt factors, for non- fully ionized complex atoms.

2. THE CALCULATION

The model refers to an atomic system, with the net charge of the core Z, and with two electrons outside closed shell, the outer 'Rydberg electron' labeled 1, being more excited than the inner electron, referred to as the 'valence electron' and labeled 2. The other electrons, [γ], are named core electrons. For example, Ba-like W^{18+} has configuration [Xe] $6s^2$, Sr-like W^{36+} has [Kr]$5s^2$, Hf-like W^{2+} has [Xe] $4f^{14}5d^26s^2$, etc. These configurations can be written as [Xe] $n_2l_2j_2n_1l_1$, for Ba-like and in a similar form for the others. The quasi-continuum states are of type $5d_{5/2}nf$ (J=5) or $6p_{3/2}nh$ in Ba-like W^{18+} with decay channel $5d_{5/2}nl \rightarrow 5d_{3/2}\varepsilon' l$ and such spectra may be grass-like in their complexity. In the present proposal these spectra are simulated in '*a single configuration description*' assuming that, the Rydberg electron evolves from a bound hydrogenic state (n_1l_1) to a continuum state (εl) while, the valence electron falls from the excited ionic state ($n_2l_2j_2$) to a lower state ($n_0l_0j_0$). The valence electron strongly interacts with the core. Hence the spin-orbit effect for this electron dominates all other interactions. The electronic repulsion $1/r_{12}$ is generally stronger than spin-orbit effects for the Rydberg electron.

Based on the Heisenberg approximation for helium [3], the 'bound' Rydberg state, $[\gamma]n_2l_2j_2n_1l_1$, has been written as zeroth-order solution for the eigenvalue equation, in the coordinate-space representation. The 'excited' Rydberg state of the atomic system, $[\gamma]n_0l_0j_0n_sl_s$, has been described in the Coulomb formalism accounting for the general properties of the Coulomb Green Function (CGF) and its Sturmian representation. In this case, the resolvent, G(Ω), of the non-relativistic Hamiltonian, $H_C = H_0 + V$, with $H_0 = p_0^2/2 + U(r_0) + p_s^2/2 - 1/r_s$ and $V = 1/r_{0s} - 1/r_s$, is a solution of the operator equation $(\Omega - H_C)\,G(\Omega) = 1$, where Ω is a complex energy variable and G is the CGF.

Assuming nonpenetration hypothesis, the valence electron is always closer to the core than the Rydberg electron, and configuration mixing arising from perturbation by interaction *V* is a small effect as long as the two wave functions are spatially separated. Then, the potential *V* can be treated as perturbation thus that, the dipole matrix elements between 'bound' and 'excited' Rydberg states, $[\gamma]n_2l_2j_2n_1l_1 \rightarrow [\gamma]n_0l_0j_0n_sl_s$, in intermediate coupling, can be written as product of two mono-electronic matrix elements. The effective oscillator strength averaged over continuous spectrum can be defined as: $f_{eff} = \dfrac{f_{eff}(n_l)}{n_l}$ where:

$$\tilde{\ }_{eff}(n_1) = \frac{2m}{3he^2} \,¥\, \frac{Es}{2J+1} \sum_{n_0,\, l_0,\, j_0,\, l_s} \sum_{n_s} \left|\langle n_2l_2j_2 | r_2 | n_0l_0j_0 \rangle\right|^2 \left| \left(\int_0^{\infty} dr R(n_1l_1;r) S(k_s,n_sl_s;r) \right) \right|^2 \tag{1}$$

In Eq. (1) the sum runs over the complete (discrete + continuous) set of eigenstates of H_C. The *'averaged excitation energy'*, $E_{s,}$ is given by: $E_s = E_{n_2l_2j_2} - E_{n_0l_0j_0} - 1/2n_l^2 = -k_s^2/2$, with $E_{n_2l_2j_2}$ and $E_{n_0l_0j_0}$ threshold energies. The $R(n_ll_l;r)$ and $S(k_s,n_sl_s;r)$ are hydrogenic and Sturmian radial components of the wave functions with respect to the valence (n_1l_1) and continuum electron (n_sl_s), respectively, *m* and *e* are the electron mass and charge, respectively, and *J* is the total angular momentum of the initial state. Finally, the G –factors for ionization of level n_1 has been evaluated as $G_l = 1 + f_{eff} \ln\left|1 + \dfrac{E4Ry}{\chi_l}\right|$, where E is the collision energy, χ_1 the ionization energy of level 1, $\chi_l = Ry/n_l^2$, and Ry =13.6eV.

3. RESULTS

In intermediate coupling, $f_{eff}(n_l)$ depends on *k* but not on *J*, since the whole Hamiltonian is independent of the Rydberg-electron spin. The effective oscillator strengths averaged over continuum for Be-like Ar and Ba-like W, ions, in dipole approximation, are given in Table1. The calculation refers to continuum states with n_s ranges from n_1 to 15.

For $1s^22p_{3/2}4d \rightarrow 1s^22s_{1/2}np$ and $1s^22p_{3/2}4p \rightarrow 1s^22p_{1/2}ns$ series in CIII, bound-free Gaunt factors and free-free Gaunt factors, are plotted versus electron temperature in Fig.1. The corresponding photon energy E_s, and effective oscillator strengths, f_{eff}, averaged over continuum, is given next to the curves. For free-free transitions, the quadrupolar term have been included in Eq.(1). In Fig.2 free-free and bound-free Gaunt factors are plotted versus electron temperature for given photon energy.

CONCLUSIONS

The accuracy of the numerical calculation depends on the accuracy of the parent ion energy calculation and on the performed infinite, but discrete, sum over n_s of term involving the overlap integral between hydrogenic and Sturmian functions. The last one has been controlled in a self-consistent manner on the basis of the partial sum rules of the averaged oscillator strengths. These rules are fulfilled only in the case when the photon frequency equals to the difference of the eigenvalue of the approximate Hamiltonian to the wave functions used in the calculation, (E_s), is substituted in the oscillator strengths, $f_{eff}(n_1)$. The parent energies have been evaluated in the MQDT/R-matrix methods[4] for C^{2+} and Al^{9+} ions, and Cowan's code for Ba-like W.

ACKNOWLEDGEMENTS

This work has been conducted under the European Fusion Development Agreement.

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ion	*transition*	$f_{eff}(n_1)$	
W^{18+}	$[Xe]\ 6p_{3/2}n_1h \rightarrow [Xe]6s_{1/2}n_sg$	*k=7/2*	*k=9/2*
	$n_1 = 6$	1.028552	0.411421
	7	1.296603	0.518641
	8	0.292346	0.116938
Ar^{14+}	$[He]\ 2p_{3/2}n_1d \rightarrow [He]\ 2s_{1/2}n_sp$	*k=1/2*	*k=3/2*
	$n_1 = 3$	0.126883	0.063441
	4	0.088255	0.044127

Table 1: The effective oscillator strengths averaged over continuum for W^{18+} and Ar^{14+}. Continuum quantum numbers n_s ranges from n_1 to 15.

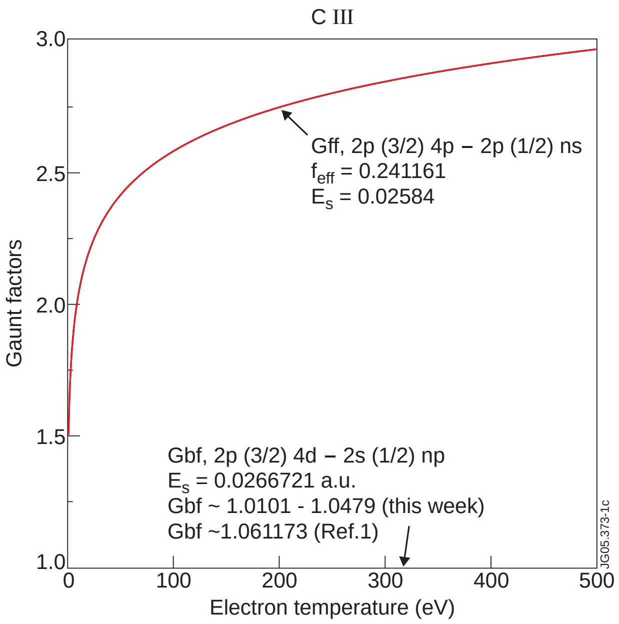

Figure 1: Bound-free (Gbf) and free-free (Gff) Gaunt factor in C^{2+}. Effective oscillator strengths averaged over continuum, f_{eff}, and photon energy, E_s, in atomic units (a.u.), are given next to the curves.

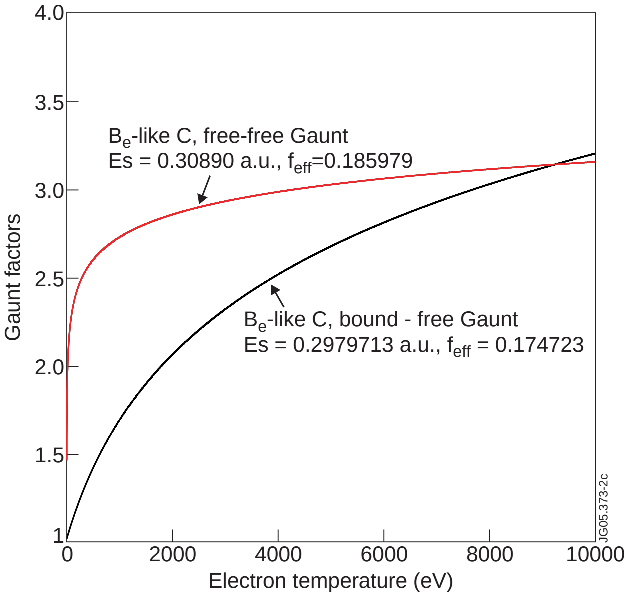

Figure 2: Gaunt factors for C^{2+} at given photon energy, E_s, in atomic units, versus T_e, in eV.