

RADIATIVE GAUNT FACTORS

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In this work we will consider the possibility of using the Coulomb Green's function for the calculation of both, bound and quasi-continuum state energy of a system with two active electrons outside closed shell. Our approach is based on the Sturmian representation of the wavefunction for the free electron. The corresponding effective quantum numbers for bound and continuum states are included into the calculations of free-free and free-bound Gaunt factors. The link to the experiments is the ability of the models to generate synthetic spectral features which can assist in analysis of observed spectra. Comparisons with other methods are also provided.

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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. 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

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coefficients are also required for thermalised electron plasmas. To have a spatially non-equilibrium balance we need to express all these coefficients by using Gaunt factors.

The present paper is mainly addressed to plasma physics community drawing attention to the uncertainty coming from atomic data calculation. The present paper's main concern is with ensuring the completeness of Gaunt factors effects in effective ionic charge modeling and not with all the consequential modeling of populations and ion distributions in plasma. The key issue then is the starting point of uncertainties in the fundamental component reaction rate coefficients. Where does the error in a fundamental reaction rate (mostly theoretical) come from? The uncertainty in collisional-radiative coefficient is a composite of uncertainties in the possibly very many contributing individual reaction.

The work proposes a new method for evaluation of bound-bound, bound-free and free-free Gaunt factors. The underlying theoretical development is the building up of a capacity for full generalized collisional-radiative modeling of many electron, heavy systems in arbitrary, possibly high, states of ionization. The model is designed to complement the models used for few electron, light systems. The link to the experiments is the ability of the models to generate synthetic spectral features which can assist in analysis of observed spectra. Particularly, we have used the Coulomb-Green's function for the calculation of both, bound and continuum state energy. The positions of atomic states are analyzed using a Sturmian expansion of the Coulomb Green's function. The method is applied to low doubly excited states of a system with two electrons outside closed shell. This representation is modified twofold. Firstly, the Sturmian term respects the same radial equation as bound-hydrogenic wavefunction. Thus, the summation on the outer – electron principal quantum number can be performed exactly; secondly, it helps to make clear the connection between the CGF formalism and a new technique which has been developed more recently in order to obtain high-order perturbative corrections to hydrogenic wavefunctions and energies. Application refers to Be-like C as an example.

2. Gaunt factors and derived atomic quantities

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]:

- a) free-free Gaunt factor:

$$g^{III} \left[(S_p L_p) \kappa \lambda SLJ, (S_p' L_p') \kappa' \lambda' SL' J' \right] \quad (1)$$

- b) free-bound Gaunt factor:

$$g^{II} \left[(S_p L_p) \kappa \lambda SLJ, (S_p' L_p') \nu' \lambda' SL' J' \right] \quad (2)$$

- c) bound-bound Gaunt factor:

$$g^I \left[(S_p L_p) \mu \lambda SLJ, (S_p' L_p') \nu' \lambda' SL' J' \right] \quad (3)$$

where, $S_p L_p$ denote the spin and orbital quantum numbers of the state γ (that is the parent state of the $z+1$ times ionized ion), $\varepsilon, \varepsilon', \kappa, \kappa'$ 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 usual Einstein coefficients, the stimulated emission rate, the stimulated recombination coefficients and the radiative recombination coefficients, can be described in terms of Gaunt factors:

$$A_{n \rightarrow n'} = \left(\frac{16\alpha^4 c}{3\sqrt{3}\pi a_0} \right) \frac{z_0^4 g_{n,n'}^I}{n^3 n' (n^2 - n'^2)} \quad n' < n \quad (4)$$

$$B_{n \rightarrow n'} = A_{n \rightarrow n'} / \frac{8\pi h \nu^3}{c^3} \quad B_{n' \rightarrow n} = \frac{n^2}{n'^2} B_{n \rightarrow n'}$$

where, $\nu = (z_0^2 I_H / h)(1/n'^2 - 1/n^2)$ is the frequency of the $n \rightarrow n'$ photon, and $g_{n,n'}^I$ the bound-bound Gaunt factors.

The excitation rate is written as:

$$q_{n \rightarrow n'}^e = \frac{2^8}{3} \left(\frac{2\sqrt{\pi} \alpha c a_0^2}{3} \right) \frac{n^3 n^5}{(n'^2 - n^2)^4} \frac{g_{n,n'}^I}{z_0^2} \left(\frac{I_H}{kT_e} \right)^{1/2} \exp(-\Delta E_{n,n'} / kT) P(\Delta E_{n,n'} / kT_e) \quad (5)$$

and the de-excitation rate for hydrogenic ions by electrons is given by:

$$q_{n \rightarrow n'}^{(e)} = \frac{2^8}{3} \left(\frac{2\sqrt{\pi} \alpha c a_0^2}{3} \right) \frac{n^3 n^5}{(n'^2 - n^2)^4} \frac{g_{n,n'}^I}{z_0^2} \left(\frac{I_H}{kT_e} \right)^{1/2} P(\Delta E_{n,n'} / kT_e) \quad (6)$$

for $n' > n$. In general an effective P-factor is deduced from more complex collision cross-section calculations or experimental cross-section measurements.

In a similar manner the bound-free rates are obtained in terms of the bound-free Gaunt factors, $g_{n,\kappa}^II$. With a Planck radiation field of energy $u(\nu)$ at temperature T_r and dilution W , the photo-ionization rate coefficient from the level n is given by:

$$\int u(\nu) B_{n \rightarrow \kappa} d\kappa = \left(\frac{8\alpha^4 c}{3\sqrt{3}\pi a_0} \right) \frac{W z_0^4}{n^5} \int_{I_n / kT_r}^{\infty} \frac{g_{n,\kappa}^II dx}{x(e^x - 1)} \quad (7)$$

The stimulated recombination coefficient is:

$$\int u(\nu) B_{n \rightarrow \kappa} d\kappa = 8 \left(\frac{\pi a_0^2 I_H}{kT_e} \right)^{3/2} \left(\frac{8\alpha^4 c}{3\sqrt{3}\pi a_0} \right) \frac{W z_0^4}{n^3} \exp(I_n / kT_e) \int_{I_n / kT_r}^{\infty} \frac{g_{n,\kappa}^II \exp(-T_r x / T_e) dx}{x(e^x - 1)} \quad (8)$$

and the radiative recombination coefficient is defined as:

$$\alpha_n^{(r)} = 8 \left(\frac{\pi a_0^2 I_H}{kT_e} \right)^{3/2} \left(\frac{8\alpha^4 c}{3\sqrt{3}\pi a_0} \right) \frac{z_0^4}{n^3} \exp(I_n / kT_e) \int_{I_n / kT_e}^{\infty} \frac{g_{n,\kappa}^II \exp(-x) dx}{x} \quad (9)$$

where, $I_n = z_0^2 I_H / n^2$, T_e is the Maxwellian free electron temperature.

The local photon emissivity $\varepsilon(\lambda)$ at a given wavelength is written as:

$$\varepsilon(\lambda) = n_e n_i Z_{\text{eff}}^2 \bar{g}(\lambda, T_e) \left(\frac{e^2}{4\pi\epsilon_0} \right)^3 \frac{8\pi}{3\sqrt{3} m_e^2 c^3 h} \left(\frac{2m_e}{\pi k T_e} \right)^{1/2} \exp\left\{ -\frac{hc}{kT_e \lambda} \right\} \frac{1}{\lambda} \quad (10)$$

$\varepsilon(\lambda)$ is given in units of [photons / s . sr . m³ . Å].

The only thing that changes when bremsstrahlung is treated quantum mechanically is the Gaunt factor.

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 a pair-coupling, jk , scheme ($J_i + l = K$ and $K \pm 1/2 = J$, where J_i is the total angular momentum of the target state, l is the orbital momentum of the added electron and $1/2$ its spin) Gaunt factor is written as follows:

$$g(k_i, k_{i'}) = \frac{2\sqrt{3}}{\pi} \sum_{l, l'} \langle l \rangle \left| \int F_{k_i l_i} F_{k_{i'} l_{i'}} \frac{dr}{r^2} \right|^2 \quad \text{where } L_i + S_i = J_i, \quad J_i + l_i = K \text{ and } K_s = J^T. \quad (11)$$

3. Method of calculation

Our proposal is to consider the possibility of using the Coulomb Green's function for the calculation of both, bound-free and free-free Gaunt factors. The method has been suggested from the multiphoton calculations where there are three different representations of the Coulomb Green's function: momentum space representation, co-ordinate space representation and Sturmian representation. The last one is dated 1970 when Hostler [5] derived so-called Coulomb Sturmian functions.

Our approach is based on the Sturmian representation of the wavefunction for the free electron. The advantage of using this representation is coming from the fact that the Sturmian term respects the same radial equation as bound-hydrogenic wavefunction. Thus, the summation on the outer – electron principal quantum number can be performed exactly. The radial components of the Coulomb Sturmian functions are solutions of the equation:

$$\left[\frac{1}{r^2} \frac{d}{dr} r^2 \frac{d}{dr} - \frac{l(l+1)}{r^2} - x^2 \right] S_{n,l,x}(r) = -2nx \frac{1}{r} S_{n,l,x}(r) \quad (12)$$

where, the parameter x , $\text{Re } x > 0$ is kept fixed and n is a positive integer. Accordingly, for $x = (-2\Omega)^{1/2}$, they provide a natural expansion basis for $G_1(r, r'; E_s)$.

Besides a normalisation constant, the radial Sturmian functions have a structure similar to those of bound-state hydrogenic functions:

$$S_{n,l,x}(r) = N_{n,l}(x) \exp(-xr) (2xr)^l L_{n-l-1}^{2l+1}(2xr) \quad (13)$$

where, L_{n-l-1}^{2l+1} are Laguerre polynomials and the normalisation factor reads

$N_{n,l}(x) = \frac{2x}{\sqrt{Z}} \sqrt{\frac{(n-l-1)!}{(n+1)!}}$. The expansion of G_1 over the Sturmian basis reads explicitly:

$$G_1(r, r'; \Omega) = \sum_{n=l+1}^{+\infty} \frac{S_{n,l,x}(r) S_{n,l,x}(r')}{1 - n/\tau} \quad (14)$$

A few specialized analytical expressions in terms of hypergeometric functions of several variables are available for three-photon dipole transition amplitude. These formulae have been derived with the help of the results obtained for the second-order perturbative corrections to a given hydrogenic wavefunction. More general (multiple-) integral representations have also been derived and again, the Sturmian approach reveals itself to be more useful in computations [6]. The N -photon amplitude is written as an $(N-1)$ -order sum running over discrete Sturmian states. A typical N -order radial component entering the general transition amplitude equation associated to an N -photon transition from state $|n_0, l_0\rangle$ to $|n, l_N\rangle$ reads:

$$M_{n,l_N/n_0l_0}^{(N)} = \sum_{v_{N-1}} \sum_{v_{N-2}} \dots \sum_{v_1} \frac{\langle R_{n_N l_N} | r | S_{v_{N-1}, l_{N-1}} \rangle \langle S_{v_{N-1}, l_{N-1}} | r | S_{v_{N-2}, l_{N-2}} \rangle \langle S_{v_{N-2}, l_{N-2}} | \dots \langle S_{v_1, l_1} \rangle \langle S_{v_1, l_1} | r | R_{n_0 l_0} \rangle}{(1-v_{N-1}x_{N-1})(1-v_{N-2}x_{N-2}) \dots (1-v_1x_1)}$$

where $x_J = \sqrt{-2\Omega_J}$, $|R_{n,l}\rangle$ are radial hydrogenic wavefunctions, $|S_{v,J}\rangle$ are radial Sturmian components, and the Sturmian index obeys $v_J \geq l_J + 1$ with $l_J = l_{J-1} \pm 1$.

The dipole matrix elements $\langle S_{v_J, l_J} | r | S_{v_{J-1}, l_{J-1}} \rangle$, between Sturmian and/or hydrogenic radial components are always reducible to a combination of hypergeometric polynomials, which can be computed to within any chosen accuracy.

4. Results. System with 4 electrons: $1s^2 n_2 l_2 n_1 l_1$ (Be-like)

We consider a system with 4 electrons: a closed shell core plus two active electrons, named valence electron with $n_2 l_2 j_2$ and Rydberg electron with $n_1 l_1$ quantum numbers. The proper description of a such system is a pair-coupling scheme: $J_i + 1 = K$ and $K + 1/2 = J$, where J_i is the total angular momentum of the target state, l is the orbital momentum of the added electron and $1/2$ its spin. In the case of photoionisation of CIII, the main resonances are those of $1s^2 2pns \ ^1P^0_1$ and $1s^2 2p \ d^1P^0_1$. Following Bethe and Salpeter [7] the Hamiltonian for a such system can be written as:

$$\begin{aligned} H &= H_0 + V \\ H_0 &= \frac{p_2^2}{2} + U(r_2) + \frac{p_1^2}{2} - \frac{\xi}{r_1} \\ V &= \frac{1}{r_{12}} - \frac{1}{r_1} \end{aligned} \quad (15)$$

$\xi = 1$ for alkaline-earth atoms, but isoelectronic sequences may be considered as well.

In the perturbation expansion, the solution of this Hamiltonian is: $E = E^{(0)} + E^{(1)} + E^{(2)}$ where :

$$E^{(0)} = E(n_2 l_2 j_2, n_1 l_1) = E_{n_2 l_2 j_2} - \frac{\xi^2}{2n_1^2} \text{ is unperturbed energy; } E_{n_2 l_2 j_2} \text{ being the parent-ion energy.}$$

The first order shift $E^{(1)}$ is obtained after multipolar expansion of V (i.e.(first-order) configuration mixing):

$$\begin{aligned} E^{(1)} &= \sum_{\lambda \geq 1} \Omega(l_2 j_2 l_1; l_2 j_2 l_1; k, \lambda) \langle n_2 l_2 j_2 | r^\lambda | n_2 l_2 j_2 \rangle \langle n_1 l_1 | r^{-\lambda-1} | n_1 l_1 \rangle \\ \Omega(l_2 j_2 l_1; l_1 j_0 l_s; k, \lambda) &= (-1)^{k-\lambda-1/2} [l_2, j_2, l_1, l_0, j_0, l_s]^{1/2} \\ &\times \begin{pmatrix} l_2 & \lambda & l_0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_1 & \lambda & l_s \\ 0 & 0 & 0 \end{pmatrix} \begin{Bmatrix} l_2 & \lambda & l_0 \\ j_0 & 1/2 & j_2 \end{Bmatrix} \begin{Bmatrix} l_1 & \lambda & l_s \\ j_0 & k & j_2 \end{Bmatrix} \end{aligned} \quad (16)$$

The second order shift: both electrons are in perturbing state ($n_0 l_0 j_0, \nu l_s$) implies a sum over the principal quantum numbers of the perturbing state (n_0, ν) including the discrete and continuum part of the spectrum. However, the sum over n_0 may usually be restricted to a discrete and even finite one:

$$E^{(2)} = \sum_{\substack{n_0 l_0 j_0 \\ l_0 \geq 1}} \sum_{\substack{\lambda_1 \geq 1 \\ \lambda_2 \geq 1}} \langle n_2 l_2 j_2 | r^{\lambda_1} | n_0 l_0 \rangle \langle n_0 l_0 j_0 | r^{\lambda_2} | n_2 l_2 j_2 \rangle \times \Omega(l_2 j_2 l_1, l_0 j_0 l_s; k, \lambda) \Omega(l_2 j_2 l_1, l_0 j_0 l_s; k, \lambda_2) \times \sum_{\nu} \langle n_1 l_1 | r^{-\lambda_1 - 1} | \nu l_s \rangle \frac{1}{E_s - E(\nu)} \langle \nu l_s | r^{-\lambda_2 - 1} | n_1 l_1 \rangle \quad (17)$$

where the denominator is:

$$E_s - E_{\nu} = E(n_2 l_2 j_2, n_1 l_1) - E(n_0 l_0 j_0, \nu l_s) \quad (18)$$

and 'Coulomb Green's function energy' is given by:

$$E_s = E_{n_2 l_2 j_2} - E_{n_0 l_0 j_0} - \frac{\xi^2}{2n_1^2}$$

and $E(\nu) = -\xi^2/2\nu^2$ for a discrete state and any positive number for a continuum state.

We will assume the net charge $\xi = 1$; otherwise, it is easy to state that the first order hydrogenic element scales as $\xi^{\lambda+1}$ while the second order involved in $E^{(2)}$ scales as $\xi^{\lambda_1 + \lambda_2}$.

We have to emphasize that $E^{(1)}$ includes the interaction of the outer electron with the core polarised by the inner electrons. One has to consider core polarisation by the outer electron: this will give rise to an additional term in energy shift; moreover, if there are quasi-degenerate states, the non-diagonal matrix elements is easy to be write. In this work we concentrate on the possibility of using Sturmian representation for calculating effective quantum numbers.

Analytical representation of Coulomb Green's function is:

$$\sum_{\nu} \langle r | \mathcal{V}_s \rangle \frac{1}{E_s - E(\nu)} \langle \mathcal{V}_s | \nu \rangle = G(r, r'; E_s) = \frac{k\Gamma(l_s + 1 - \kappa)}{rr'} M_{\kappa l_s + \frac{1}{2}}(2r_{<}/\kappa) W_{\kappa l_s + \frac{1}{2}}(2r_{>}/\kappa) \quad (19)$$

$$E_s = -1/2\kappa^2 = -k_s^2/2$$

The product of Whittaker functions has an integral representation in terms of modified Bessel function. Starting from the relation:

$$\langle n_1 l_1 | r^{-\kappa-1} | k_s ; n_s l_s \rangle = \int_0^{\infty} dr r^{-\kappa+1} R(n_1 l_1; r) S(k_s, n_s l_s; r) \quad (20)$$

where,

$$R(n_1 l_1; r) = N(n_1 l_1) r^{l_1} e^{-r/n_1} F(l_1 + 1 - n_1; 2l_1 + 2; \frac{2r}{n_1})$$

$$S(k_s, n_s l_s; r) = N(k_s, n_s l_s) r^{l_s} e^{-k_s r} \times F(l_s + 1 - n_s; 2l_s + 2, 2k_s r) \quad (21)$$

$$N(n_1 l_1) = \frac{2}{n_1^2} \frac{(2/n_1)^{l_1}}{(2l_1 + 1)!} \left(\frac{(n_1 + l_1)!}{(n_1 - l_1 - 1)!} \right)^{1/2}$$

$$N(k_s, n_s l_s) = \frac{(2k_s)^{l_s+1}}{(2l_s + 1)!} \left(\frac{(n_s + l_s)!}{(n_s + l_s - 1)!} \right)^{1/2}$$

The matrix element between hydrogenic and Sturmian wavefunction is written as:

$$\langle n_1 l_1 | r^{-\kappa-1} | k_s, n_s l_s \rangle = N(n_1 l_1) N(k_s, n_s l_s) \times \frac{(2l_1 + 1)!}{\left(k_s + \frac{1}{n_1}\right)^{l_1 + l_s - \kappa + 2}} \times \sum_{p=0}^{n_1 - l_1 - 1} \binom{n_1 - l_1 - 1}{p} \frac{(l_1 + 1 - \kappa + p + 1)!}{(2l_1 + p + 1)!} \times \left(\frac{-2/n_1}{k_s + 1/n_1} \right)^p \times F \left(l_s + 1 - n_s, l_1 + l_s - k + p + 2, 2l_s + 2; \frac{2k_s}{k_s + \frac{1}{n_1}} \right) \quad (22)$$

It can be seen that the needed dipole radial matrix elements have structure similar to the well known Gordon formula for dipole matrix elements between hydrogenic bound states. The sum can be recast in the form of a Taylor-like series expansion

The hypergeometric function $F(a, b, c; z)$ has a general expression valid for any m and n integer, α and z complex, such that $1-z$ is not a negative real number:

$$F(-\alpha, m+1, n+1; z) = \frac{(-1)^{n-m} n! (1-z)^{\alpha+n-m}}{m! (\alpha+1)_n z^n} \left[\sum_{p=0}^m \binom{m}{p} (n-m)_{m-p} (\alpha+1)_p z^p \right] + (-1)^{m+1} \frac{n!}{m!} \sum_{p=m+1}^n \frac{(-1)^p (p-m)_m z^{-p}}{(n-p)! (\alpha+1)_p} \quad (23)$$

where, $\binom{n}{m}$ is the binomial coefficient $= \frac{n!}{(n-m)!m!}$ and a_n is the Pochhammer symbol $= 1$ if $n=0$ and $a(a+1)\dots(a+n-1)$ for positive integer n . If $m > n$ the second term is absent and the first sum ranges from $p = n$ to m .

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.

Our results for effective quantum numbers are in very good agreement with those reported by more sophisticated method in the Ref. 8. Table 1 shows part of these results:

Table 1. Effective quantum numbers relative to 2S ionization threshold.

state	this work	Ref.8.
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

We have implemented the above discussed method to output values of bound-free Gaunt factors for 3p-ns and 3p-nd series in CIII. Results are given in Figs.1 and 2.

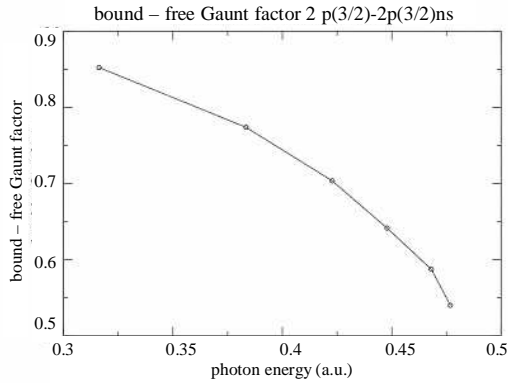


Fig. 1.

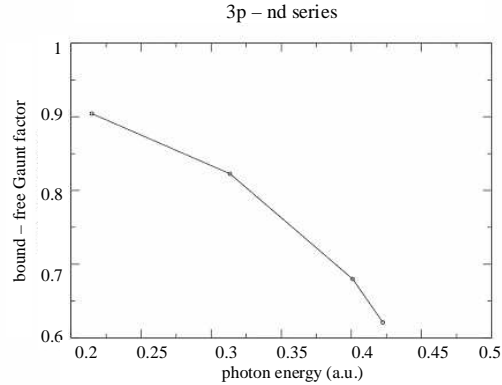


Fig. 2.

5. Conclusions

In the present work we have considered the possibility of using the Sturmian representation of the wave function and Coulomb Green's function in energy to calculate effective quantum numbers and Gaunt factors for a system with four electrons. The present formalism is unable to derive the threshold energies, therefore in computations the experimental values would be welcome.

As a results, one must consider the present work as a calculation of quantum defect rather than energies. By representing the continuum states in the Sturmian representation, a new technique more efficient, with same accuracy or better than R-matrix can be implemented to calculate atomic data for complex atoms in plasma. 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 [9].

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 improved 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 [10]; our results for effective quantum numbers are in very good agreement with those reported by K. Berrington in the Ref. 9.

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