INVESTIGATION OF DISCREPANCIES IN THE Zeff MEASUREMENTS MADE AT JET

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Background

For some time there has been a discrepancy between Zeff as measured by the charge exchange system and the visible continuum spectrum. The aim of this collaboration is to probe possible reasons that may contribute to resolving the discrepancy and use this information to improve the routine data analysis.

Deliverables

Reconciliation between the two methods of measuring Zeff on JET and a technique for keeping both diagnostic systems synchronized.

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Problem: *Location of any free-bound edges and effect of using a mean Gaunt factor or species mix for background bremsstrahlung*

This task has been considered under and outside Campaigns C8-C14

Methods:

a) *semi-empirical calculation* based on the quantum defect method to determine the asymptotic series expansions of radial wave functions in the pure Coulomb regime; The radial integrals can therefore be evaluated semi-empirically in so far as they are dominated by the long –range Coulomb part without detailed knowledge of the short-range non-Coulomb atomic potential. The radial integrals have been evaluated in this manner by Bates & Damgaard (1949) for the bound-bound case, by Burgess & Seaton (1960) for the bound-free case, and by Peach (1965,1967) for the free-free case. It is observed that the radial integrals are approximately sinusoidal functions with phase $\pi(\mu - \mu' + \chi)$ where χ is slowing varying.

b) Effective potential numerical method can be expected to improve the calculations. The adopted Slater type potential (Burgess& Summers1987) is:

$$V(r) = \frac{z_0}{r} - \sum_{i=1}^{s} \frac{q_i}{r} \exp\left(-\frac{\alpha_i z_i r}{n_i}\right) r^{n_i} \left(\sum_{k=0}^{n_i} a_{ik} r^{-k} \right)$$

The electron in shell *i* is supposed to be screened from the nucleus by the electrons in shells < *i* and partially screened by the other electrons in the shell *i* itself.

c) New proposal is to consider the possibility of using the Coulomb Green's function (CGF) for the calculation of both, bound-free and free-free Gaunt factors. Our approach

is based on the Sturmian representation of the wavefunction for the free electron. The advantages of using the Sturmian approach are: firstly, the Sturmian term respects the same radial equation as the bound-hydrogenic wavefunction. Thus, the summation on the outer – electron principal quantum number can be performed exactly; secondly, the old routines for evaluating bound-free or free-free Gaunt factors could be used without any modification. The importance of this representation is twofold. On the one hand, it can be used to implement efficient schemes to compute N-photon amplitudes with N ≥ 2; *on the other hand, it helps to make clear the connection between the CGF formalism and new techniques which have been developed more recently in order to obtain high-order perturbative corrections to hydrogenic wavefunctions and energies.*

Computational implementation:

The stringent calculation of the free-free Gaunt factor, which is a quantum mechanical correction factor for the emitted bremsstrahlung, is very computationally heavy.

- The effective potential can be regarded as an improvement of the calculation. The final result of the correction to the decay rate of $2s_{1/2} - 1s_{1/2}$ transition seems to be $-2.025(1)\,[\alpha(Z\alpha)^2/\pi]\,\log[1/(Z\alpha)^2]$
- Semi-empirical calculation uses LS coupling –not an appropriate coupling scheme

We have implemented the new formalism to calculate radiative Gaunt factor for a system with four electrons. *The proper description of such a system is a pair-coupling scheme*: $J_i + l = K$ *and* $K + ½ = J$. *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.*

In the case of photoionisation of CIII, the main resonances are those of $1s^2 2pns\ {}^1P^0_1$ and $1s^2 2p\,nd\,{}^1P^0_1$. 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.

The radial components of the Coulomb Sturmian functions are solutions of the equation:

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

where the parameter *x, 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 $G_l(r,r';E_s)$.

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

$S_{n,l,x}(r) = N_{n,l}(x)\exp(-xr)(2xr)^l L^{2l+1}_{n-l-1}(2xr)$, where L^{2l+1}_{n-l-1} are Laguerre polynomials and the normalisation factor reads $N_{n,l}(x) = \dfrac{2x}{\sqrt{Z}}\sqrt{\dfrac{(n-l-1)!}{(n+1)!}}$

The needed dipole radial matrix elements have structure similar to the well-known Gordon formula for dipole matrix elements between hydrogenic bound states (Gordon'29). The sum can be recast in the form of a Taylor-like series expansion.

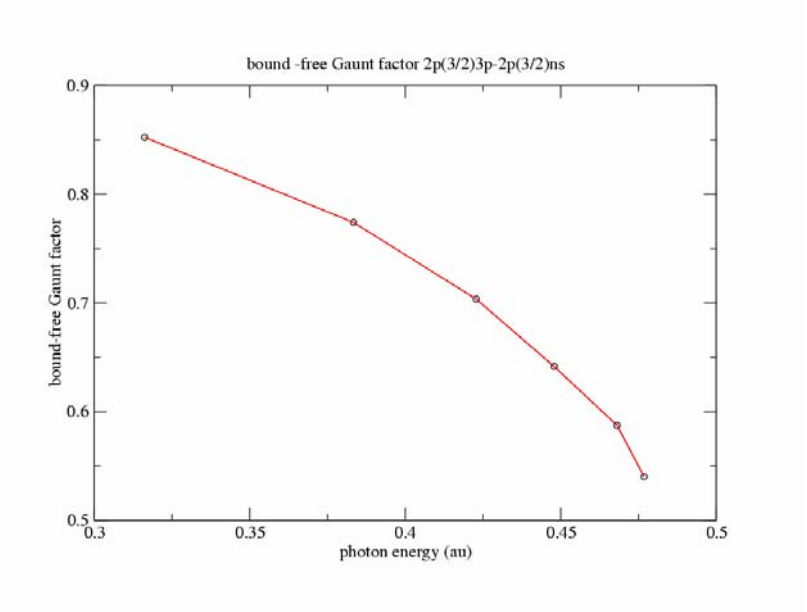

Figure1

In the Figure 1 are presented our preliminary results concerning the bound-free Gaunt factor calculated with respect to the photon energy (in atomic units) for $2p_{3/2}3p - 2p_{3/2}ns$ series in CIII ion.

Our preliminary results on bound-free Gaunt factors were compared with those calculated using the old methods. Conclusions can be summarized as follows:

a) the work should be continued to have more results and comparisons with other methods; these first results are considered the better ones at this moment. (before February 2004)

b) the new formalism was considered more economic comparing with other methods (R-matrix) and will be implemented on ADAS baseline as a new routine for faster calculations of the excited Rydbergs states effective quantum numbers.

c) a new FORTRAN routine will be written to calculate the Gaunt factor; to evaluate Zeff by theoretical methods and to compare this with the results of the JET diagnostic KS3

d) a paper will be devoted to this work before February 2004