ATOMIC DATA FOR OPEN d -SHELL ELEMENTS

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1. Overview

The aim of the project is to provide

1. atomic data for the open d-shell elements, and
2. the strategy for implementing an ITM (software) capacity for AMNS data (ITM-09-TFL2-AMNS-T2, ITM-09-TFL2-AMNS-T3)

The ITM has identified a broad need for data relating to atomic, molecular, nuclear and surface physics data (AMNS). Since the uses of the data within the ITM are quite wide-ranging, a consistent approach taking into account the specific requirements of the ITM, while maintaining the effort aligned with other European efforts in this area, is required. The AMNS group has been implemented as a Task under the TF leadership to identify and report, in collaboration with the relevant ITM projects (ISIP), on the detailed ITM needs for AMNS data, to propose a strategy for implementing an ITM (software) capacity for AMNS data taking into account existing European efforts in this area and to act as a response group suggesting short term solutions for the ITM.

AMNS data are needed in several of the ITM modelling projects, but especially in IMP#3 and IMP#5. A consistent approach, taking into account the specific requirements of the ITM while maintaining the work aligned with other European efforts in this area, is therefore required.

A significant amount of atomic data (not always easily accessible) is needed. It will take a significant amount of time and effort before the bulk part of the needed data can be made available in the ITM-TF. The short term needs can be summarised as follows : Rate coefficients (as a function of n and T) for: ionization, recombination, charge-exchange, nuclear reaction rates,cooling rates,ionization potential, energy per nuclear reaction + fraction of it going to electron and ion components (this is to a large part a question for IMP#5). The elements needed are: High priority (needed in 2008/09): H, D, T, He, C; Since the ADAS database is very well established and contains data essential to several ITM-TF codes, it will be used as a pilot project to import atomic data to the ITM-TF data repository.

The work on providing the AMNS data includes recommendation of the best data to be used/stamp of approval. Highly useful data is residing in data bases not readily accessible to the general user (e.g. in private data bases). With the access to such data, we will supply, when appropriate, relevant data to the ITM-TF database. This will include suggesting recommendation for the best data to be used.

The first requirement in any scattering calculation is a good representation of the target, i.e. accurate wave functions for the target ion. Such representation usually requires the inclusion of configuration interaction (CI) in the atomic model, which affects the calculated energy levels and oscillator strengths of the ion. Furthermore, comparisons between calculated and experimental energies and oscillator strengths of the target are important indicators of the

quality of the target representation and the overall accuracy of the obtained cross sections and collision strengths.

To this goal, the project aims to obtain accurate atomic data for Co IV ion, using the R-matrix theory and codes. These data necessary for spectral identification will be stored in a database in order to be incorporated in the ITM –TF codes. A special attention is paid to resonances in electron scattering with these ions.

Excitation can be a direct process or a result of resonant dielectronic capture followed by autoionization leaving the target ion in an excited state. Resonant enhancements to the cross section are significant in optically-forbidden transitions and can dominate the direct contribution by an order of magnitude or more near threshold. Direct configuration interaction (CI) and indirect interactions with a common continuum have shown to produce interference between nearby resonances and have a strong effect on the resonance contributions to the cross sections as calculated in the close coupling formulation. It has been found that the resonance structure is sensitive to the exact energies of the individual resonances. The increasing sophistication of collision calculations carried out over the last years has depended to a considerable extent on rapidly increasing power of the supercomputers available to such research.

The difficulties in theoretical calculations of these processes come from the interference effects between the direct and the indirect processes. One approximation widely used to treat these phenomena is the Distorted Wave Born approximation (DWBA) Following this approximation the intermediate resonance state is independent of its decay. A second approximation uses the R-matrix method to evaluate excitation cross section to the autoionizing states. In this case the interference effects with the direct process are neglected. The R-matrix method with one suitably chosen pseudo-state (RMPS) to represent continuum electrons accurately includes both direct and indirect processes as well as the interference effects between them. As in the CCC approach, this method approximates the effects of higher-lying discrete and target continuum states by a set of pseudostates, which are incorporated into the R-matrix programs.

The present work suggests two approaches that offer a partial solution to these problems. The first of these is the single-photon reaction approach. The second one is the inclusion of scattering states in the R-matrix approach. Section 2 gives detailed results from general investigation of high lying single-particle state in one-photon transfer reaction. They are to be compared with the two-particle-one-hole resonance effects in electron scattering with open d-shell Co IV ion. Section 3 gives our concluding remarks.

2. Detailed Results

2.1. High-lying single particle states in one-photon transfer reaction.

The high-lying single-particle states, in one-photon transfer reaction, manifest themselves as broad ‘resonance’-like structures superimposed on a large continuum. The R-matrix Floquet (RMF) theory and code has been very successful in describing in stationary state the atomic structure properties as well as photo-ionization and electron-impact excitation processes, especially in the near-threshold resonance regime.The general investigation, which started with studies of $\Delta n = 0$ channels [1] and extended for $\Delta n = 2$ channels [2] for the $1s^2 2pns(^1P^0) \rightarrow 1s^2 2sn's(^1S^e)$ transitions in Li-like Al and C ions, has been indentified as potential candidates for achieving the partial rates of one –photon detachment as direct response to an exchange of character that occurs between the ‘bound’ Rydberg and the ‘resonant’ Rydberg state as the two states are swept through resonance.

- [1] V. Stancalie, **Physics of Plasmas. 12** (2005).
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As, it is a non-perturbative approach, whose accuracy is, in principle, only limited by the number and the quality of the target states accounted for in the expansion including the coupling to the continuum. This representation consists, in principle, of bound states, outgoing resonance, and a limited number of scattering states along a path in the complex energy plane corresponding to a general one-body potential. Using such a basis one would obtain the same results as those obtained by any standard methods used to calculate quantities along the real energy axis. However, quantities that are evaluated on the complex plane, like partial decay width (which are defined as the residues of the S matrix) can provide complex physical quantities.

The proper description of electron scattering from open shell ions must involve an adequate description of electron correlation as well as radiation damping. This problem has been solved a number of times using different tools. In the presence of an attractive Coulomb field one has infinite series of resonances. Further complications can arise if one has overlapping resonances. In a simple picture the strength of a resonance (integrated cross section) is proportional to the ratios $\Gamma^r\ \Gamma^a/\ (\Gamma^r + \Gamma^a)$, where Γ^r and Γ^a are the radiative and autoionization transition probabilities, respectively. If Γ^a and Γ^r are comparable in size the strength gets smaller. This is commonly called radiation damping. For Li-like ions in recombining plasma regimes, the di-electronic recombination process is mainly due to the capture of free electrons by ions in $1s^22s$ and $1s^22p$ configurations, producing autoionizing Be-like levels, which emit a photon to give bound levels of $1s^22snl$ and $1s^22pnl$ configurations. The basic process of interest is:

$$e^- + X^{Z+}(1s^2 2s(^2S^e)) \Leftrightarrow X^{(Z-1)+**}(1s^2\ 2p\ n'\ l'(\ ^1P^0)) \rightarrow X^{(Z-1)+*}(1s^2 2s\ n''l'\ (^1S^e)) + h\nu \qquad (1)$$

The incident electron is captured by the Li-like ion into a doubly excited resonant state, which can decay, either by electron emission or by photon emission. In the latter case the resultant ion state can be a bound state and hence we have recombination. In the above equation X^{Z+} signifies the Li-like ion, of nuclear charge Z, in its ground state, and $X^{(Z-1)+**}$ is the doubly excited state of the corresponding Be-like ion of nuclear charge (Z-1). This state can decay by radiative transition to other excited state $X^{(Z-1)+*}$. Owing to the electron temperature during the recombination phase in plasma (≤ 200 eV), the most probably ways involve the autoionizing levels $1s^22pnl\ ^{1,3}L'_{J'}$ and $1s^23pnl\ ^{1,3}L'_{J'}$ (with initial ion $1s^22s$) and $1s^23dnl\ ^{1,3}L'_{J'}$ (with initial ion $1s^22p$). They can be characterized respectively by the core transitions 2s – 2p, 2s – 3p and 2p – 3d.

Let consider the reverse process of single-photon ionization. Following this approach, the doubly excited Rydberg state, $1s^22pns(^1P^0)$, and the Rydberg excited state $1s^22sns(^1S^e)$ in equation (1), are dressed by a laser field assumed to be monochromatic, monomode, linearly polarized and spatially homogeneous. The attention is restricted to monochromatic laser field of angular frequency $\omega = \Delta E$ (the transition energy corresponding to the initial unperturbed – field free- Rydberg states) and an intensity given (as an appropriate guess) by the electric field strength of the 2s –2p core transition. Results are analyzed within the two-state model which qualitatively reproduced the behavior of the Floquet states, showing that the coupling via the continuum is more important than the direct dipole coupling between states.

When only a single resonant process occurs, either in the limit that the laser intensity goes to zero so that only the autoionizing resonance remains, or in the limit that the width of the

autoionizing state goes to zero, leaving only the 'capture- escape' resonance, the ratio of the scattering cross section to the background cross section reduces to the Fano line shape formula. The Fano resonance formula is algebraically simple. A dimensionless energy ε is used to measure energy differences from a resonance energy E_r in terms of the half-width. For an *isolated* autoionization state with a resonant width Γ at resonant energy E_r, the resonant structure can be described in terms of the asymmetry parameter q. This parameter is a measure of the importance of the direct transition from the ground to the continuum compared to transition via the autoionizing state. High q means weak direct transition and symmetric line shape since the interference is minimized. Qualitatively, the q parameter measures the interference between transitions from the initial state to the bound and continuum components of the final-state wave function. If the resonance is dominated by the contributions from the transitions to both bound and continuum components of the final-state wave function, its corresponding q value is generally large and the resonant feature is approximately symmetric. If the contributions from transitions to bound and continuum components of the final-state wave function are comparable, the resonant structure is asymmetric with an intermediate q value. If the spectrum is strongly dominated by the transition to the continuum component of the final-state wave function, a *window resonance* with zero cross section is expected either at or near the resonant energy E_r with $q \to 0$.

In Fig. 1 the ratio $R = (q+\varepsilon)^2/(1+\varepsilon^2)$ is plotted as function of relative energy parameter and different q values for the $1s^2 2pns(^1P^0)$, n =5 state in CIV. The relative energy has been determined as $\varepsilon = \lfloor 2(E_g + \hbar\omega - E_a \rfloor / (\Gamma_a + \gamma_a - \Gamma_g)$, where E_g, ω, and E_a are, respectively, the field free position of the excited Rydberg state, the tuning frequency and the field-free position of the autoionizing state, as output from the R-matrix Floquet calculation.

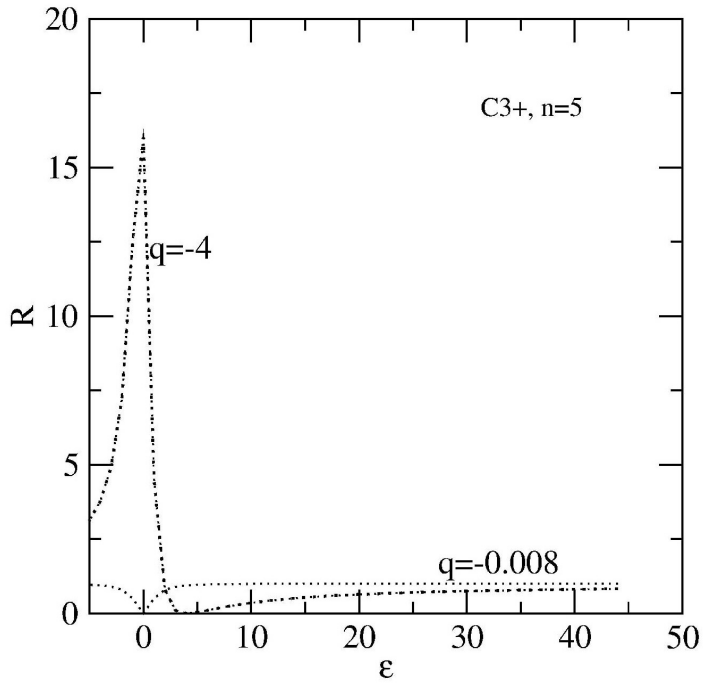

Figure 1: Line profile ratio for $1s^2 2p5s$ ($^1P^0$) resonant state in C^{2+} as function of the relative energy parameter in atomic units(a.u.)

The first step of this damping process is usually described as the coupling of the single particle state with core field. In the following steps, coupling to more sophisticated configurations may

occur until the system reached a completely equilibrated stage, i.e. a compound atomic system. Emission of a particle can occur at each stage of this damping process. The total width Γ of the decaying state is usually written as the sum of two contributions referred to as the 'escape width' and the 'spreading width' respectively. The escape width is related to the direct process, e.g. a fast photon emission either immediately after the primary excitation process or during the first step of the damping process. The spreading width is related to 'electron evaporation' from the compound atomic system whose corresponding decay channels can be predicted by statistical model calculation.

2.2. Two-Particle-one-hole resonances in electron-collision with open-d shell elements

In this section we present results of a series of calculations intended specifically to explore the role of resonances in scattering process in the vicinity of 3d threshold of Al^{10+}, and 3d threshold of Fe-peak element Co IV.
These resonances can be associated with S-matrix poles lying on an unphysical energy sheet just below each threshold and can therefore be interpreted as nuclear-excited Feshbach resonances. The role of the long-range dipole interaction is also discussed. The results indicate that the use of accurate target eigenstates and a more accurate treatment of the collision problem may change the cross sections by as much as 20% from earlier work.
The process under consideration in Co IV ion is as follows:

$$\begin{aligned} e^- + \quad Co^{3+}\left(3p^6 3d^6\, {}^5D\right) \rightarrow Co^{2+*} \quad & \left(3p^5 3d^8, 3p^5 3d^7 4s, or\, 3p^5 3d^7 4p\right) \\ \downarrow & \\ Co^{3+} \quad & \left(3p^6 3d^6, 3p^6 3d^5 4s, or\, 3p^6 3d^5 4p\right) + e^- \end{aligned} \tag{2}$$

The intermediate Co IV resonance states ($3p^5 3d^8$, $3p^5 3d^7 4s$ and $3p^5 3d^7 4p$) are referred to as 'two-particle-one-hole' states. Here electron attachment goes along with electronic excitation of the target atom so that two electrons occupy previously unoccupied orbitals and a hole is left in one of the lower lying atomic orbitals. Such resonances are also denoted as core-excited resonances.

In order to study the effect on two-particle-one-hole resonance in electron collision with Fe-peak element Co IV, the atomic structure calculation has been initiated. In this LS-coupling calculation, the 136 states arising from the $3d^6$, $3d^5 4s$ and $3d^5 4p$ configurations of Co IV have been retained. The accuracy of a series of models for the target terms was considered, which form the basis of *R*-matrix collision calculations. The 136 target states have been represented by elaborate configuration interactions in an attempt to account for electron correlation effects where it is essential to include the $3p^2 \rightarrow 3d^2$ core excitation in both the target and scattering wave functions. The internal region solution is obtained using the RMATRXII program package. In the external region, the program FARM has been used for comparison at some scattering energies. This work provides a firm foundation on which larger calculations may be based.
The increasingly sophisticated e^- - Co^{3+} calculations that have been carried out are summarized as follows:

Calculation A: 3-state *LS* –coupled R-matrix calculation. First, we included in the R-matrix expansion all 136 LS coupled states which arise from the three target configurations $3d^6$, $3d^5 4s$ and $3d^5 4p$. In the present level of approximation, in order to have a balanced configuration interaction representation for the 136 *LS*-coupled Co IV target states and the associated scattering wave functions, we began our calculations by employing the Hartree-Fock orbitals of the $1s^2 2s^2 2p^6 3s^2 3p^6 3d^6\ ^5D$ ground state configuration augmented with two spectroscopic orbitals, namely, the 4s and 4p; Calculation B: 6-state *LS* –coupled R-matrix calculation. We included in the R-matrix expansion all 136 *LS* coupled states which arise from six target configuration $3d^6$, $3d^5 4s$, $3d^5 4p$, $3p^4 3d^8$, $3p^4 3d^7 4s$ and $3p^4 3d^7 4p$ looking at the effect of configuration interaction. All these 136 states are represented by multi-configuration interaction wave functions and include the two-electron core excitation $3p^2$ –> $3d^2$ configurations in the target wave functions; Calculation C: 9-state *LS* –coupled R-matrix calculation. Starting with the 136-level model, we included in the R-matrix expansion all 136 *LS* coupled states which arise from nine target configuration $3d^6$, $3d^5 4s$, $3d^5 4p$, $3p^4 3d^8$, $3p^4 3d^7 4s$, $3p^4 3d^7 4p$, $3p^5 3d^7$, $3p^5 3d^6 4s$ and $3p^5 3d^6 4p$. The 136 target states have been represented by elaborate configuration interactions in an attempt to account for electron correlation effects where it is essential to include the $3p^2 \rightarrow 3d^2$ core excitation in both the target and scattering wave functions. To allow for the accurate representation of terms of $3d^5 4d$ it was necessary to optimize 4d physical orbital on ^7D level.

The number of continuum basis functions included in each channel was set to 20 to give accurate results for incident electron energies up to 16 Ryd. Finally, the collision strengths have been calculated for total angular momentum values L = 0 – 12 which gave good convergence for all the transitions considered in this paper.
Figure 2 gives collision strengths as obtained from the first calculation (calculationA). Results refer to ^5D - ^3P forbidden transition which gives the dominant contribution to cross section. Figure 3 shows the modified collision strengths due to the presence of intermediate states included explicitely in (N+1) wave function expansion. The role of configuration interaction due to $3p^2$ – $3d^2$ two electron promotion included into the target model is illustrated for the considered ^5D - ^3P forbidden transition. This is to be compared with Figure 1. Finally, Figure 4 shows the role of two-particle one-hole resonances on the collision strengths.

Separate calculation has been done for Al^{10+} to be compared. In this case, two different target model calculations have been done. In the first calculation (CalculationA) the only six target states have been included into the N-electron wave function expansion: $1s^2 2s$, $1s^2 2s$, $1s^2 2p$, $1s^2$ 3s, $1s^2 3p$ and $1s^2 3d$. In the calculation B, these states were increased with the next eight $1s^2 4s$, $1s^2 4p$, $1s^2 4d$, $1s^2 4f$, $1s^2 5s$, $1s^2 5p$, $1s^2 5d$, $1s^2 5f$, 1nd $1s^2 5g$. Comparison of these two calculations is given in figures 5 and 6 where the corresponding collision strengths are plotted versus electron collision energy (in Rydberg).

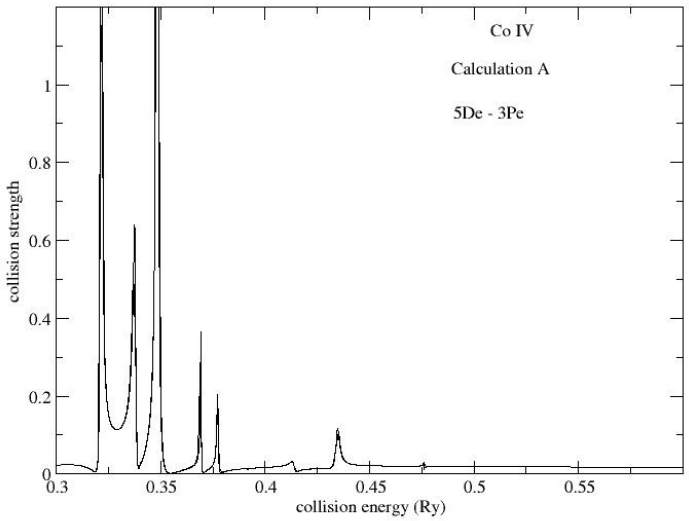

Figure 2: Collision strength for the $^5D^e$-$^3P^e$ forbidden transition in Co^3. The curve corresponds to the first calculation without the intermediate states included in the(N+1)-electron atomic system wavefunction expansion

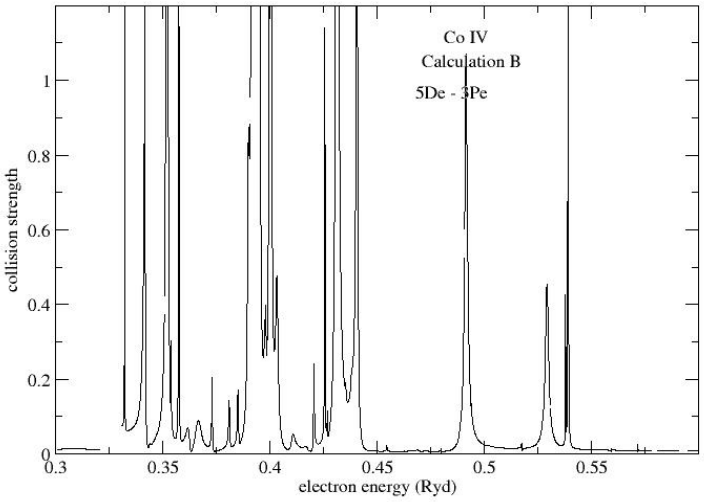

Figure 3: Collision strength for the $^5D^e$-$^3P^e$ forbidden transition in Co^3. The curve corresponds to the second calculation with the intermediate states included in the (N+1)-electron atomic system wavefunction expansion

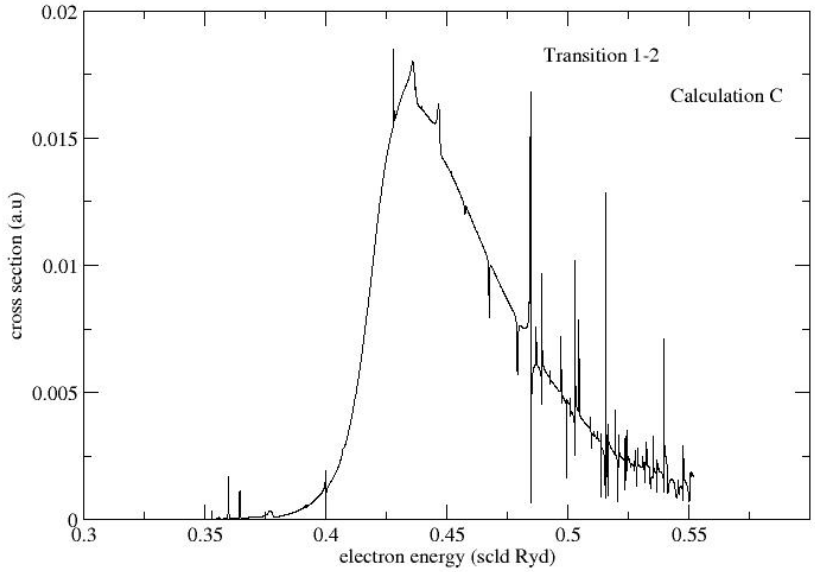

Figure 4: Collision strength for the $^5D^e$-$^3P^e$ forbidden transition in Co^3. The curve corresponds to the third calculation with the intermediate states included in the N+1 wvefunction expansion. Nine target states were been included into the N-electron wave function description. The role of two-particle-one-state resonances is illustrated comparing with results from Figure 3.

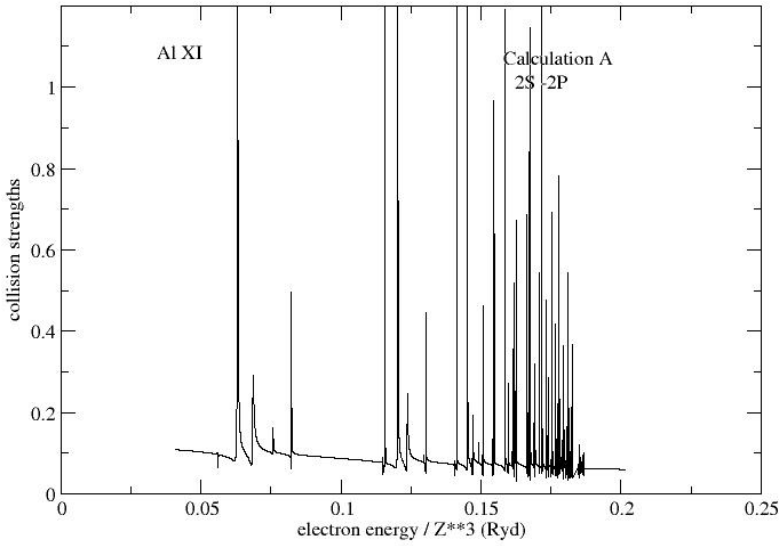

Figure 5: Collision strength for the $^2S - ^2P$ transition in Al^{10+}. The curve corresponds to the first calculation with six target states included into the model.

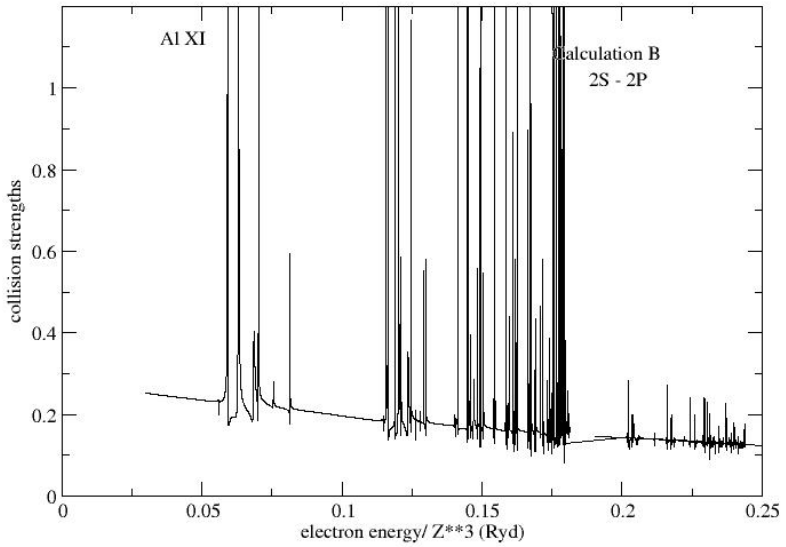

Figure 6: Collision strength for the $^2S - ^2P$ transition in Al^{10+}. The curve corresponds to the second calculation with 14 target states included into the model.

3. Concluding remarks

We have initiated different electron collision calculation in order to determine the atomic data for complex ions Co^{3+}, Z = 27, total number of active electrons 24. The calculation provided energy levels, transition probabilities and oscillator strengths. A special attenstion has been paid to resonance phenomena which can affect the plasma parameters. These processes have been studied comparing different target models included in electron-scattering calculation. Results obtained can be summarised as follows: a) for ions with small number of electrons (Li-like is an example) the inclusion of intermediate states into the (N+1)-electron atomic system wave function does not provide information on resonance structure and damping phenomena. In this case the analysis should be done with more sophisticated models as photoionization and laser assisted processes.b) for Fe-peak elements as Co^{3+} the inclusion of intermediate states into the (N+1)-electron atom wave function provides a firm foundation on which larger calculations may be based.

Publications:

[1] V. Stancalie, " *On Rydberg series of autoionizin resonances"* **Nuclear Instruments and Methods B:** 267 (2009) 305 – 310.

[2] V. Stancalie, "*Theoretical atomic data calculation foor plasma spectroscopy"* **Laser and Particle Beams** 27 (2009) 345- 357.