Studies on the Electron-Correlation and Relativistic Effects in Target Representation and Low-Energy Collision Calculation

V. Stancalie, C. Iorga and V. Pais

National Institute for Laser, Plasma and Radiation Physics, Magurele - Ilfov, Romania

Exploring the importance of including CI wave functions in the target –state expansion and in the (N+1)-electron quadratically integrable function expansion

I. **Fe-peak CoIV (Cr-like) : Z=24 : $3p^6(^2D^e)$**   Phys. Scr. **83** (2011)025301

The accuracy of a series of models for the target terms has been investigated including all of the 136 LS-coupled states, arising from the three manifolds $3d^6$, $3d^54s$, $3d^54p$ in the *R*-matrix expansion.

a) **3-state LS –coupled R-matrix calculation, Calculation A.** First, we have included in the R-matrix expansion all 136 LS coupled states which arise from the three target configurations $3d^6$, $3d^54s$ and $3d^54p$.

b) **6 –state LS** –coupled R-matrix calculation, Calculation B, retains also 136 LS terms arising from the three configurations above augmented with $3p^43d^8$, $3p^43d^74s$ and $3p^43d^74p$ in the target state expansion and the configurations $3p^53d^8$, $3p^43d^9$,$3p^43d^84s$ and $3p^53d^54s^2$ in the (N+1)-electron quadratically integrable function expansion.

c) New target states to represent the 136 Co IV energies from the $3d^6$, $3d^44s$, $3d^44p$ levels by allowing double electron promotions from the 3p-shell into the 3d-shell and single electron promotion into the **4s, 4p and 4d** –shell: 272 LS terms of the four configurations $3d^6$, $3d^54s$, $3d^54p$ and $3d^54d$ are included in the *R*-matrix expansion.

$$e{-} + Co^{3+}(3p^63d^6\ ^5D) \rightarrow Co^{2+*}(3p^53d^8, 3p^53d^74s\ or\ 3p^53d^74p)$$
$$\downarrow$$
$$Co^{3+}(3p^63d^6, 3p^63d^54s\ or\ 3p^63d^54p) + e{-}$$

Exploring the effect of electron correlation in the target representation and collision calculation

I. Fe-peak CoIV (Cr-like) : c) **9-state LS-coupled** R-matrix calculation,Calculation C, shows the effect on the collision strengths of including additional 48 levels with electronic configuration $3p^53d^7$. In this calculation the target states were represented by $3d^6$, $3d^54s$, $3d^54p$, $3p^43d^8$, $3p^43d^74s$ and $3p^43d^74p$, $3p^53d^7$, $3d^44s^2$ and $3d^44s4p$, and correspondingly the (N+1)-electron configurations $3p^63d^7$, $3p^63d^64s$, $3p^63d^64p$, $3p^63d^64s^2$, $3p^63d^54s4p$, $3p^53d^8$, $3p^43d^9$, $3p^43d^84p$, $3p^43d^74s4p$, $4p^53d^74p$, $3p^43d^74p^2$, $3p^53d^44s4p$ and $3p^53d^64p^2$

Single Excitation from 3d	Double Excitation from 3d	Single Excitation from 3p	Double Excitation from 3p
$3d^54s$	$3d^44s^2$	$3p^53d^7$	$3p^43d^8$
$3d^54p$	$3d^44s4p$	$3p^53d^64s$	$3p^43d^74s$
$3d^54d$	-	$3p^53d^64p$	$3p^43d^74p$

II. Mg-like S^{4+}: $2p^63s^2$ ($^1S_0$)

ADNDT: http://dx.doi.org/10.1016/j.adt.2016.06.002

A.   Ch. F.Fisher (2006)

I. Reference configurations: $1s^22s^22p^6$ ($3s^2$, $3s3p$): single and double excitation from the valence electrons to account for the valence correlation effect

II. Reference configurations $2s^22p^6\{3s^2,3p^2,3d^2\}$ and $2s^22p^6\{3s3p,3p3d\}$ allowing one 2p electron and one valence electron excitation

III. Similar but allows one 2s electron to be excited

II + III account for 2p and 2s core-valence correlation effect

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B. Present

$1s^22s^22p^6 (3snl, 3pnl, 3dnl)$ $1 \leq n \leq 7, 0 \leq l \leq 4$ $\rightarrow$ 567 fine-structure levels
$1s^22s^22p^53s^2 nl$,
$1s^22s^22p^53s3p\ nl$, $1 \leq n' \leq 5, 0 \leq l \leq 4$ $\rightarrow$ 2580 fine-structure levels
$1s^22s^22p^53p^2 nl$

ε	valence-valence	valence-valence + valence-2p core correlation
ε_λ	0.43%	0.28%
ε_A	3.7%	3.1%
ε_I	4.1%	3.4%

$$R_{ul} = \frac{I_{obs} \times N_E \times \lambda_{ul}}{(N_{ul} / N_{S^{4+}}) \times A_u}$$

Table A The transition dependent scattered electron energy for different transitions concerning the excitation from the first four fine-structure levels. ε is given in Rydberg units.

Lower level	Upper level		
ε	0.00012	0.022	0.089
1	2–6	7–567	
2	3–4	5–14	15–567
3	4	5–14	15–567
4		5–14	15–567

Coll. Strengths comparison:
FAC-DW :   UCL-DW

Exploring the importance of including relativistic effects in the target representation and low-energy electron collision calculation
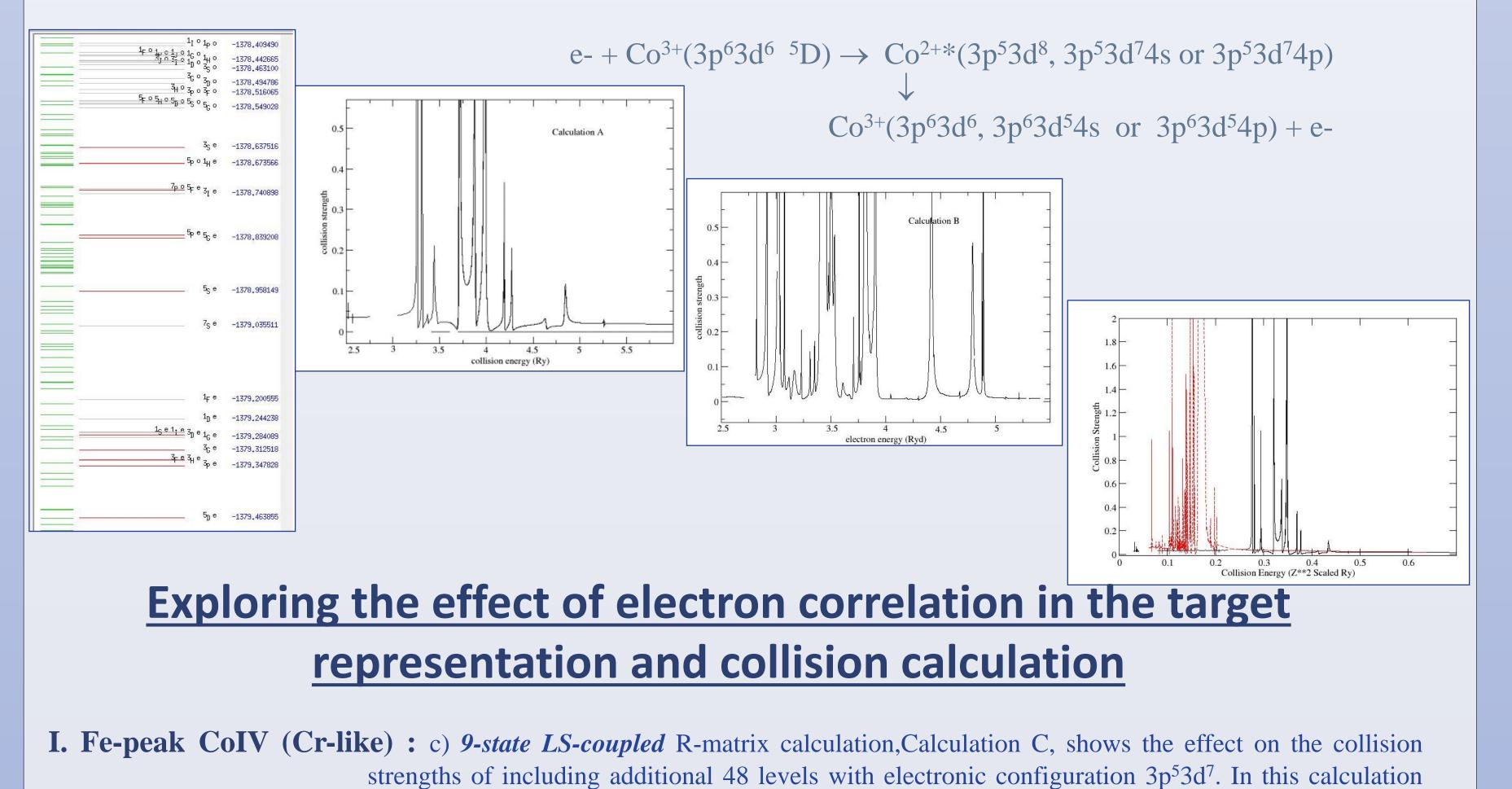
I. **Fe-peak Cr-like Co IV**   ADNDT**107**(2016)140-220

FAC1: 1334 levels among the $3d^6$, $3d^54l$, $3p^53d^7$, $3p^43d^8$, $3p^33d^9$, and $3p^23d^{10}$ levels

FAC2: 21.992 levels of the $3d^6$, $3d^54l$, $3d^55l$, $3p^63d^44l4l'$,$3p^53d^7$ and $3p^43d^74l$ configurations

FAC3: FAC2+37 198 levels of the $3p^43d^8$, $3p^33d^9$,$3p^23d^{10}$, $3p^63d^45l5l'$ and $3p^43d^75l$ configurations

FAC4: FAC3 +12 338 levels of the $3p^53d^64l$ and $3p^53d^55l$ configurations

FAC5: FAC4 + 4610 levels of the $3p^33d^84l$, $3p^23d^94l$, and $3p3d^{10}4l$ configurations.

76 138 levels included in CI: Discrepancies with NIST up to **35%** for the majority of levels

GRASP: 21 configurations $3d^6$, $3d^54l$, $3d^55l$, $3d^44l^2$, $3d^44l4l'$ and $3p^53d^7$: 14 732 levels

14.732 levels included in CI: Significant discrepancies with NIST up to **26%** for some levels

QRHF : radial orbitals (RO) are calculated quasi-relativistic Hartree -Fock and are supplemented with the transformed radial orbitals (TRO) for $5 \leq n \leq 8$ and all possible l (Bogdanovich et al. CPC 2002,2005).
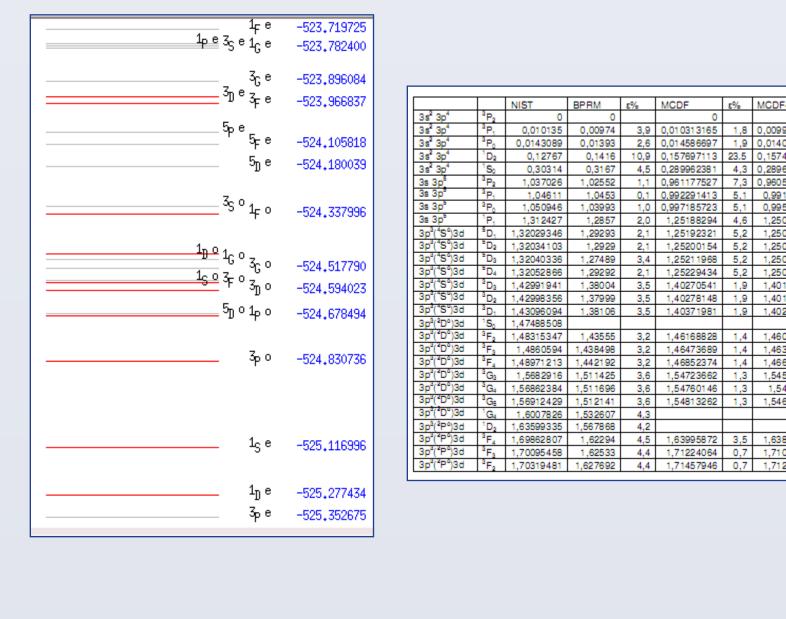
1 563 846 levels included in CI with the QRHF code:Discrepancies with NIST less than **3%** for some levels
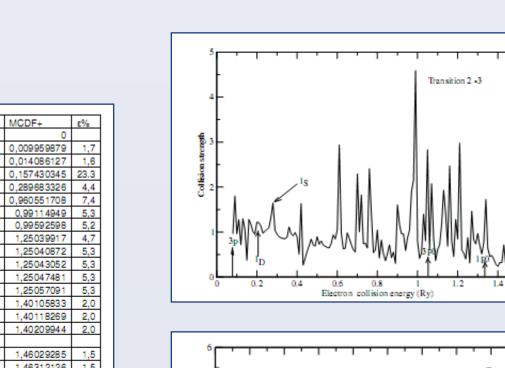
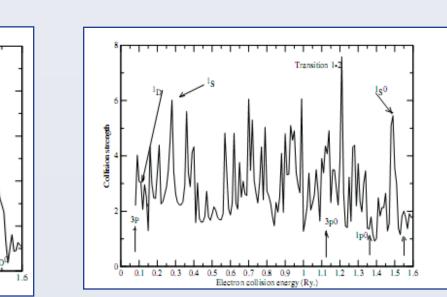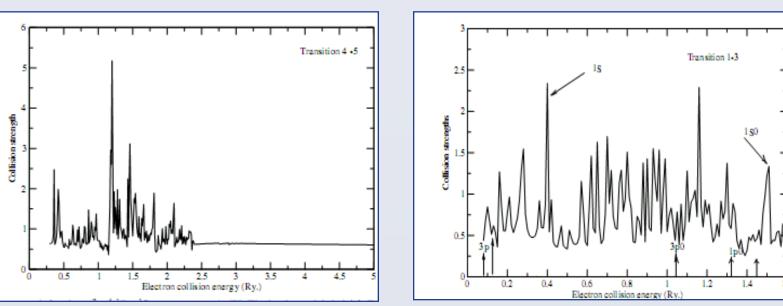**II.** **S-like Ar $^{2+}$**   Eur. Phys. J. D **66**(2012) 84

BPRM: CI limited to single and double excitations within n=3 complex; GRASP: J^π: $0^\pm$, $1^\pm$, $2^\pm$,3^-,4^-,5^-. 24 terms arising from the configurations: $3s^23p^4$, $3s3p^5$, $3s^23p^33d$ and $3p^6$ for both BPRM and MCDF calculations

$$e^- + Ar^{2+}(3s^23p^2\ ^3P) \rightarrow Ar^{2+*}(3s^23p^5, 3s^23p^43d, 3s3p^6, 3s3p^53d, 3s^23p^33d^2,\ or\ 3s3p^43d^2)$$
$$\downarrow$$
$$Ar^{2+}(3s^23p^4, 3s3p^5, 3s^23p^33d,\ or\ 3s3p^43d)$$

III. **Mg-like S^{4+}**   AIP Conf. Proc, APiP Conf. Aprile 2016, Paris

Collision calculation has been performed keeping constant the target states number in the R-matrix expansion (the lowest 17 target states) for the ICFT and MCDF/DARC approaches

Rates comparison:
FAC-DW
UCL-DW

Detailed quantitative description of the level population kinetics in plasmas

Can. J. Phys. **93** (2015) 1413-19

➢ XUV emission from the autoionizing levels in Al XI observed at the interaction of high intensity, short pulse laser with Al target at nhelix test-bed facility at GSI;
➢ Modeling of radiative decay rates for the high order intercombination transitions

1s2/2l' autoionizing levels   **1s2/3l' autoionizing levels**   **Two electron transitions**

Intercombination transitions   **High order two-electron transitions**

High order intercombination transitions