Theoretical study of electron-impact ionization in atoms and ions

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Outline

• Theory

• Single ionization
  • Convergence of the excitation-autoionization (EA) cross sections
  • Resonant excitation double autoionization (REDA)
  • Correlation effects
  • The scaled DW cross sections

• Conclusions
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• **Theory**

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Single ionization by electron impact

\[ \sigma_{if}(\varepsilon) = \sigma_{if}^{\text{DI}}(\varepsilon) + \sigma_{if}^{\text{indir}}(\varepsilon) \]

\[ \sigma_{if}(\varepsilon) = \sigma_{if}^{\text{DI}}(\varepsilon) + \sum_k \sigma_{ik}^{\text{EXC}}(\varepsilon) B_{kf}^a(\varepsilon) \]

Autoionization branching ratio:

\[ B_{kf}^a(\varepsilon) = \frac{A_{kf}^a}{\sum_n A_{kn}^a + \sum_{m<k} A_{km}^r} \]

\( A^a \) – Auger transition probability,
\( A^r \) – radiative transition probability
The scaled DW cross sections

• DI for atoms:

$$\sigma_{if}^{\text{DI}*}(\varepsilon) = \frac{\varepsilon}{\varepsilon + I + \varepsilon_k} \sigma_{if}^{\text{DI}}(\varepsilon)$$

*I* is the ionization energy, $\varepsilon_k$ is the kinetic energy of the bounded electron

• DI for ions:

$$\sigma_{if}^{\text{DI}*}(\varepsilon) = \frac{\varepsilon}{\varepsilon + I} \sigma_{if}^{\text{DI}}(\varepsilon)$$

• Excitation:

$$\sigma_{if}^{\text{EXC}*}(\varepsilon) = \frac{\varepsilon}{\varepsilon + \Delta E_{if} + \varepsilon_b} \sigma_{if}^{\text{EXC}}(\varepsilon)$$

$\Delta E_{if}$ is the transition energy, $\varepsilon_b$ is the bounding energy of electron
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$W^{17+}$ single ionization


$EA: \begin{align*}
    4s, 4p & \rightarrow nl \ (4 \leq n \leq 25), \\
    4d & \rightarrow nl' \ (5 \leq n \leq 25), \\
    4f & \rightarrow nl' \ (10 \leq n \leq 38),
\end{align*}$

where $l' \leq 5$.

$W^{17+}: 4f^{11}$
$W^{27+}$ EA channels: convergence

$W^{27+} : 4d^{10}4f$

EA : $4s,4p, 4d; n \leq 40, l \leq 6$

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DC: $4s^2 4p^6 4d^{10} + e \rightarrow \begin{cases} 4s 4p^6 4d^{10} n_1 l_1 n_2 l_2 \\ 4s^2 4p^5 4d^{10} n_1 l_1 n_2 l_2 \end{cases}$

$n_1 = 4, 5, n_2 = 4 - 40, l_1 l_2 < 5$
Se$^{3+}$

DC: $3d^{10}4s^24p + e \rightarrow 3d^94s^24p \ n_1 l_1 n_2 l_2$

$n_1 = 4 - 6, n_2 = n_1 - 50, l_1 l_2 < 5$

Pakalka et al, PRA 97, 012708 (2018)
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Correlation effects: $W^{5+}$

$W^{5+} \ 4f^{14}5s^2 \ 5p^6 \ 5d$

$n \leq 12$

Jonauskas et al, PRA 100, 062701 (2019)
Correlation effects: $W^{5+}$

$W^{5+} \ 4f^{14} 5s^2 \ 5p^6 \ 5d$

$W^{5+} \ 4f^{14} 5s^2 \ 5p^5 \ 5d^2$

$W^{5+} \ 4f^{13} 5s^2 \ 5p^6 \ 5d^2$

$W^{5+} \ 4f^{14} 5s^2 \ 5p^6 \ 6s$

Jonauskas et al, PRA 100, 062701 (2019)
Correlation effects: Fe$^{3+}$

Influence of correlation effects

Kynienė et al, PRA 100, 052705 (2019)
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Scaling of DW cross sections: C

Exp: Brook et al 1978, J. Phys. 11, 3115

Jonauskas, AA 620, A188 (2018)
Scaling of DW cross sections: C⁺

$C^+ \ 2s^2 \ 2p$


Jonauskas, AA 620, A188 (2018)
DW cross sections: $N^+$

Experiments:
Scaling of DW cross sections: N⁺

Experiments:
Scaling of DW cross sections: N⁺

Experiments:
Conclusions

• Convergence of the EA cross sections has to be studied to provide reliable data for single ionization process.

• Resonant excitation double autoionization can produce important contribution at the lower energies of electrons.

• Correlation effects diminish single ionization cross sections.

• The scaled DW cross sections can be important in the analysis of the measurements for the neutral atoms and near neutral ions.
Thank you!