Theoretical study of electron-impact ionization in atoms and ions

Valdas Jonauskas
Institute of Theoretical Physics and Astronomy, Vilnius University, Lithuania

Electron impact ionization can be classified into direct and indirect ionization processes. Direct ionization occurs when an electron is ejected from the atomic system practically instantaneously. In contrast, the indirect process involves additional steps that lead to single ionization. For example, excitation autoionization, which is often the strongest indirect process, is initiated by electron excitation, followed by decay through Auger transition. The autoionization branching ratio is used to estimate the population transferred from the autoionizing state to the next ionization stage. Thus, the branching ratio is zero for states below the single ionization threshold.

The distorted wave (DW) approximation often overestimates single ionization cross sections for neutral atoms and near-neutral ions compared to experimental data. To address this issue, it was previously suggested to use scaling factors for the plane wave Born approximation in the study of excitation. We have extended this idea to the DW approximation by using different energy-dependent scaling factors for the cross sections of collisional ionization and excitation processes.

The study of the single ionization process must include an analysis of the convergence of the EA channels, the contribution from resonant excitation double autoionization (REDA), and the influence of correlation effects. For neutral atoms and near-neutral ions, the scaling of the DW cross sections must be incorporated in the analysis to explain experimental data.

The estimation of the convergence of EA cross sections is essential to obtain reliable data. It is meaningless to achieve good agreement with experimental data if the convergence of the EA channels is not evaluated. Previous studies have demonstrated that calculations must include excitations up to shells with a principal quantum number approximately $n = 40$ to achieve a good agreement with measurements for W^{17+}. Moreover, further studies on the W^{25+}, W^{26+}, and W^{27+} ions revealed that the inclusion of the excitations to higher shells ($n > 8$) increases the EA cross sections by a factor of two.

The REDA process provides a significant contribution to the cross sections at lower energies of impacting electrons. The inclusion of REDA cross sections improved the data for Sn4+ and Se3+ ions, resulting in a good agreement with experimental measurements.

The correlation effects can be significant in the study of the single ionization process, particularly for lower ionization stages. For instance, previous research has shown that the inclusion of the correlation effects in the analysis for the W^{5+} ion led to a reduction in single ionization cross sections. However, it should be noted that experimental data were explained by incorporating contributions from the long-lived levels of the W^{5+} ion into the model.

Previous analyses of single ionization cross sections for the C atom and C^{+} ion showed a good agreement with measurements when using the scaled DW approximation, whereas the unscaled DW cross sections were higher than the measurements. The scaled DW approximation is applied to investigate the N^{+} ion, which is planned to be analyzed in this CRP. Our current study of the N^{+} ion, which incorporates energy-dependent scaling factors for the DW cross sections, agrees well with available experimental data.