Theoretical electron-impact excitation cross sections of H, He and Li atoms

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Excitation of atoms and ions by electron impact is very important process in plasma physics modelling. However, the experimental data for electron-impact excitation cross sections are very insufficient and still possess a high degree of uncertainty, therefore imposing a need of theoretical data.

We have developed computer codes to calculate electron-impact excitation cross sections exploring different wavefunction bases using Born approximation. To evaluate the performance of these codes, several light atoms, namely H, He and Li, were chosen because there are verified data for them in NIST database [1]. Two different radial orbital basis sets were chosen for calculations, a non-relativistic (HF) and a quasirelativistic (QR) set. In case of helium and lithium, correlation effects were taken into account by using the transformed radial orbital method [2,3]. However, since the main cross section data from NIST [4] were additionally scaled, the same energy-scaling procedure was performed in our calculations. The one-configuration Dirac-Fock method (DF) was applied in [4], therefore their results were scaled using the experimental values of corresponding oscillator strengths. In current work, a multiconfiguration method is used, therefore no additional scaling is needed and our data are pure theoretical results.

We see a very close agreement with data from [4] in almost every case. Our calculated cross sections have such relative mean-square deviations: for hydrogen - $1s \rightarrow 2p$, 3p and 4p 0.22% both HF and QR; for helium - $1s^2 \rightarrow 1s2p$ 1,2% HF and 2.6% QR, $1s^2 \rightarrow 1s3p$ 3.7% HF and 4.2% QR; lithium - $1s^22s \rightarrow 1s^22p$ 1.5% HF and 1.2% QR, $1s^22s \rightarrow 1s^23p$ 35% both HF and QR. The atoms under consideration have low nuclear charges, therefore the HF and QR results are very close to each other. Our results agree better with those from [4] than any other results given in [1]. The only major difference appears in lithium $1s^22s \rightarrow 1s^23p$ excitation where further investigation is required to establish a source of discrepancies.

Overall results indicate that our employed methods and codes use are suitable to produce reliable data for excitation of light atoms by electron-impact. In future we will place these collision data together with energy level spectra and transition parameters in currently developed atomic database ADAMANT.

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