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Calculation of excitation and ionization processes using relativistic CCC method¹

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The recently formulated relativistic convergent close-coupling (RCCC) method has been applied to electron scattering from quasi-one electron atoms [1] and also highly charged hydrogenlike ions [2]. In the latter case it has been used to resolve discrepancies between theory and experiment for the polarization of x-rays emitted by hydrogenlike ions (Ti^{21+} , Ar^{17+} , Fe^{25+}) during electron impact excitation and make predictions for cross sections and radiation polarization for hydrogen-like uranium ion. Here we report on the extension of the RCCC method to accommodate electron scattering from two electron targets and quasi-two electron targets. We apply the theory to electron scattering from mercury which serves as a testing ground for relativistic theories due to its high atomic number, $Z = 80$. Furthermore, electron-mercury scattering plays an important practical role in the physics of fluorescent and high intensity discharge lamps. In our calculations the mercury atom was modeled as a quasi-two electron atom consisting of two valence electrons above an inert $[\text{Xe}]4f^{14}5d^{10}$ frozen core. One- and two-electron polarization potentials have been used to model more accurately the valence-core-electrons correlations. We have calculated cross sections for electron impact excitations of mercury for a large number of transitions. Good agreement was found with our previous nonrelativistic results for the transitions that are not strongly affected by relativistic effects (e.g., $(6s6p)^1P_1^o$). For the transitions that are strongly affected by relativistic effects (e.g., $(6s6p)^3P_1^o$) we find good agreement with recent DBSR calculations [3] and available experiment.

[1] D. V. Fursa and I. Bray, Phys. Rev. Lett. **100**, 113201 (2008).

[2] C. J. Bostock, D. V. Fursa, and I. Bray, Phys. Rev. A **80**, 052708 (2009).

[3] O. Zatsarinny and K. Bartschat, Phys. Rev. A **79**, 042713 (2009).

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