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Relativistic Calculations of Electron and Positron Scattering Length for Argon

Scattering length is one of the most useful parameters used to describe low-energy electron-atom and positron-atom collisions. It is defined as a radius of a hard sphere in the zero-energy total cross section, where the sign represents the type of interaction: it is positive for repulsion and negative for attraction. Such data is mainly used in low-temperature systems such as Bose-Einstein condensate and Fermi-Dirac condensate. The calculations are done using the multi-configurational Dirac-Hartree-Fock (MCDHF) method to account for electronic correlations using the GRASP2018 package [1]. Calculations are performed for electron scattering and positron scattering. Calculations for positron may be done in two different ways: as an electron with negative energy travelling back in time and simply by treating the positron as an electron with a positive charge. Moreover, the polarization potential is added since it plays a crucial role in the long-distance electron/positron correlation which is particularly important for very small energies and leads to the proper calculation of the scattering length. Scattering length is calculated at zero energy limit by two methods: using the asymptotic behaviour of wave function and by graphical fit at the close distance to the target.
[1] C. Froese Fischer, G. Gaigalas, P. Jönsson, J. Bieroń, Comp. Phys. Comm. 237, (2019),184-187

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