Convergent Close-Coupling Calculations of Positron-Helium Collisions

This thesis is presented for the degree of Doctor of Philosophy

by

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Declaration

I declare that this thesis is my own account of my research and contains as its main content, work which has not previously been submitted for a degree at any tertiary education institution.

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ABSTRACT

The Convergent Close Coupling (CCC) method is applied, for the first time, to the scattering of positrons on helium. The helium target wave functions are obtained within various configuration interaction (CI) expansions. In the full CI expansion the two electrons are treated equally and thus all electron-electron correlations are taken into account. In the frozen-core (FC) approximation the CI expansion fixes one of the electrons to be described by a pure 1s orbital of He^+, while maintaining the required singlet and triplet symmetries. Lastly, the multi-configuration (MC) approximation relaxes the FC approximation to allow the description of the inner electron to include several low-lying orbitals and is therefore more accurate than the FC approximation. The accuracy of the target wave functions is tested by comparing the calculated energy levels with the experimental data.

Based on positron-hydrogen scattering, comprehensive close-coupling formulas for positron-helium scattering are developed. The reduced two-centre V-matrix elements are derived in momentum space for various channels. These include direct, excitation and rearrangement channels, i.e. positronium formation.

We first consider low energy positron-helium elastic scattering for energies below the positronium formation threshold of 17.8 eV. Utilizing a single-centre expansion the elastic cross section and phase shifts have been calculated as a function of the positron incident energy. The calculations agree very well with the experimental data and the variational calculations, but not previous singleor double-centre close-coupling calculations.

We then consider energies above the first ionization threshold (24.6 eV) and calculate helium elastic, excitation, fragmentation and total cross sections within the single-centre expansion approach. Good agreement with the available experimental and other theoretical results has been obtained.

The studies have proved that a single-centre expansion, with accurate target state description, can deliver accurate data of practical value over a broad range of energies. However in the low-energy region, between the positronium formation threshold of 17.8 eV and the ionization threshold of 24.6 eV, implementation of the two-centre expansion is required. We expect this work to be undertaken in the near future, based on the derivations presented in this thesis.

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