

Electron scattering from molecular hydrogen in a spheroidal convergent close-coupling formalism

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Synopsis Electron scattering from molecules is a fundamental interaction of matter and is the mechanism behind many chemical reactions. In this work we rework the ab initio Convergent Close-Coupling scattering theory into prolate spheroidal coordinates—a natural system for diatomic molecules—to present total, differential, and ionisation cross sections of electron-H₂ collisions.

The Convergent Close-Coupling (CCC) method [1] has been highly successful in calculating data for scattering on atoms at all projectile energies of interest. Beginning with electron scattering on atomic hydrogen, it has since been extended to photon, positron, and antiproton scattering, and further developed to include relativistic effects and explicit positronium formation channels.

However, until the recent application of CCC to positron-H₂ collisions [2] this method has been limited to atomic targets, owing to the significantly increased complexity of molecules. The current theoretical data is incomplete and often in disagreement with experimental data for even the simplest molecules [3].

We are currently applying the CCC formalism to electron and positron scattering from diatomic molecules in prolate spheroidal coordinates, utilising the (fixed-nuclei) Born-Oppenheimer approximation. This coordinate system is ideally suited to diatomics as it is anchored by two foci on which we place the two

nuclei. The H₂⁺ wavefunction is separable in spheroidal coordinates, just as atomic hydrogen in spherical. To our knowledge this is the first spheroidal close-coupling calculation of electron-molecule scattering.

Preliminary results show that this approach is more accurate and more efficient than its spherical counterpart at reproducing the spheroidal nature of the diatomic scattering problem. We aim to present total, differential, and ionisation cross sections for electron-H₂ collisions, complete with comparisons to the spherical implementation as well as the future direction of this molecular scattering theory.

References

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