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Elastic scattering and rotational excitation of H_2 by electron impact

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The problem of low-energy electron-impact rotational excitation of H2 has been studied in great detail over the last 60 years, due to its importance in low-temperature hydrogen plasmas and gases. Be- low 10 eV, rotational excitation comprises up to 20% of the total cross section, and below the v = $0 \rightarrow 1$ threshold (≈ 0.5 eV) it is the dominant contribution to electron energy loss. Accurate cross sections for the rotational transitions of H_2 are vital for modelling the emission spectra of astrophysical clouds, or for constructing collisional-radiative (CR) models of fusion-relevant plasmas. Up to 0.5 eV, the $N = 0 \rightarrow 2$ and $1 \rightarrow 3$ rotational excitation cross sections are well known, with good agreement between the results of electron swarm experiments, which are reproduced by several calculations. At higher energies, however, the situation is less ideal, with substantial disagreement between various measurements and calculations.

The theoretical techniques applied to this problem in the past have utilised a variety of approximations to the treatment of coupling between rovibrational levels, from the adiabatic-nuclei (AN) approximation in which the coupling is neglected, to the most accurate rovibrational close-coupling approach. However, the common factor in all previous studies is the use of model potentials in place of coupling to the closed electronically-inelastic channels. The various choices of potential can lead to differences in the calculated cross sections far more significant than the errors introduced by the AN approximation, particularly since the greatest discrepancies are at energies more than 10 times the threshold energy, where the AN approximation is accurate. What is missing from the literature are theoretical studies of low-energy rotational excitation in which the coupling to closed electronic channels is accounted for rigorously. Within the AN approximation this is feasible provided one can solve the electronic scattering problem accurately. Here we apply the molecular convergent close-coupling (MCCC) method, which in recent years has been shown to completely solve the electronic scattering problem for H_2 [1]. The results presented here are available online [2].

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