Ionisation-with-Excitation Calculations for Electron-Impact Helium Collisions within the S-Wave Model

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Write abstract.

Declaration

Write declaration.

Acknowledgements

Write acknowledgements.

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List of Abbreviations

TCS: total cross section

SDCS: single-differential cross section

DDCS: double-differential cross section

TDCS: triple-differential cross section

TICS: total ionisation cross section

CCC: convergent close-coupling

CCC(N): convergent close-coupling calculation performed with N one-electron basis states

CCC(C, N): convergent close-coupling calculation performed with C core states and N one-electron basis states

CCC(C, N, λ): convergent close-coupling calculation performed with C core states, and N one-electron basis states with exponential fall-off parameter λ

ECS: exterior complex scaling

PECS: propagating exterior complex scaling

1 Introduction

Describe utility of Electron-Impact Helium scattering processes.

1.1 Electron-Impact Helium Scattering Processes

Describe elastic, excitation and ionisation scattering processes.

Describe auto-ionisation process for excited Helium.

Describe atomic term symbols (in context of Helium), and discuss Helium states.

1.2 Experimental Review

1.3 Theoretical Review

Discuss early development of CCC method for Electron-impact Hydrogen scattering (elastic, excitation, ionisation).

Discuss extension of CCC method to three-electon systems.

Discuss challenges encountered and overcome in obtaining accurate DCS's for ionisation processes.

Discuss decision to use S-wave model.

Discuss early CCC data for Helium TICS.

Discuss PECS data demonstrating agreement with CCC data for TICS-without-excitation but not for TICS-with-excitation.

2 Theory

2.1 Convergent Close-Coupling Method for an Atomic Target

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2.1.2 Target States

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3 Results

3.1 Helium Target States

Discuss major-configuration purity of states as function of exponential fall-off.

Figure of major-configuration purity for doubly-excited states.

Discuss interference of doubly-excited and continuum states (auto-ionisation).

Figure of Helium energy spectrum(s) and auto-ionisation threshold.

Discuss improvements in fidelity of target states and increase in computational cost with increasing number of core states.

3.2 Total Ionisation-without-Excitation Cross-Sections

Discuss agreement of CCC and PECS data for TICS-without-excitation.

Figure of CCC and PECS data for TICS-without-excitation.

3.3 Total Ionisation-with-Excitation Cross-Sections

Discuss difficulty associated with the small magnitude of TICS-with-excitation.

Figure of elastic, TICS-with-excitation and TICS-without-excitation, demonstrating magnitude difference.

Discuss how convergence is attained in multi-parameter setting (increasing the number of core states for a fixed number of one-electron basis states).

Figure of TICS-with-excitation for increasing number of core states, demonstrating convergence.

Discuss sensitivity of TICS-with-excitation to exponential fall-off parameter / target state fidelity.

Figure of TICS-with-excitation for varying exponential fall-off demonstrating variation.

Discuss difficulty in removing pseudoresonances from TICS-with-excitation.

Discuss decreasing magnitude TICS-with-excitation up to a certain number of one-electron-basis states, and increasing magnitude past this point. Mention how it may be similar to variations with exponential fall-off parameter, being affected by fidelity of target states.

Figure of TICS-with-excitation for increasing number of one-electron basis states, demonstrating suggestion of convergence in magnitude then also failure to converge.

4 Conclusion

Todo list