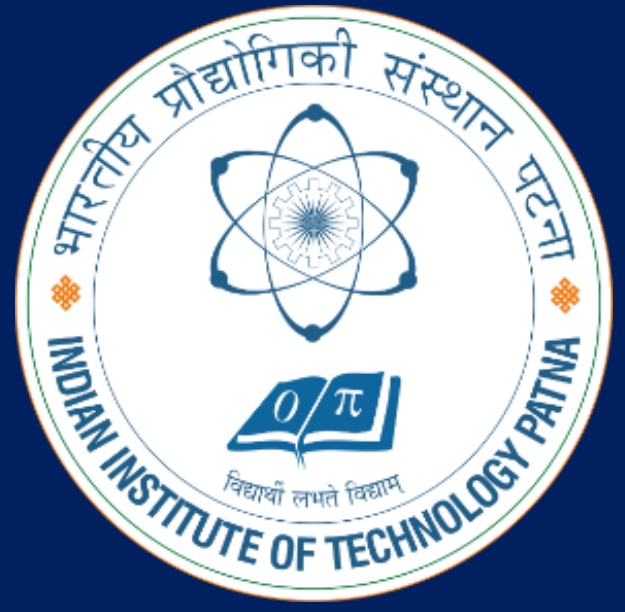


Elastic electron scattering from alkali earth metals- analysis using MCDF approach

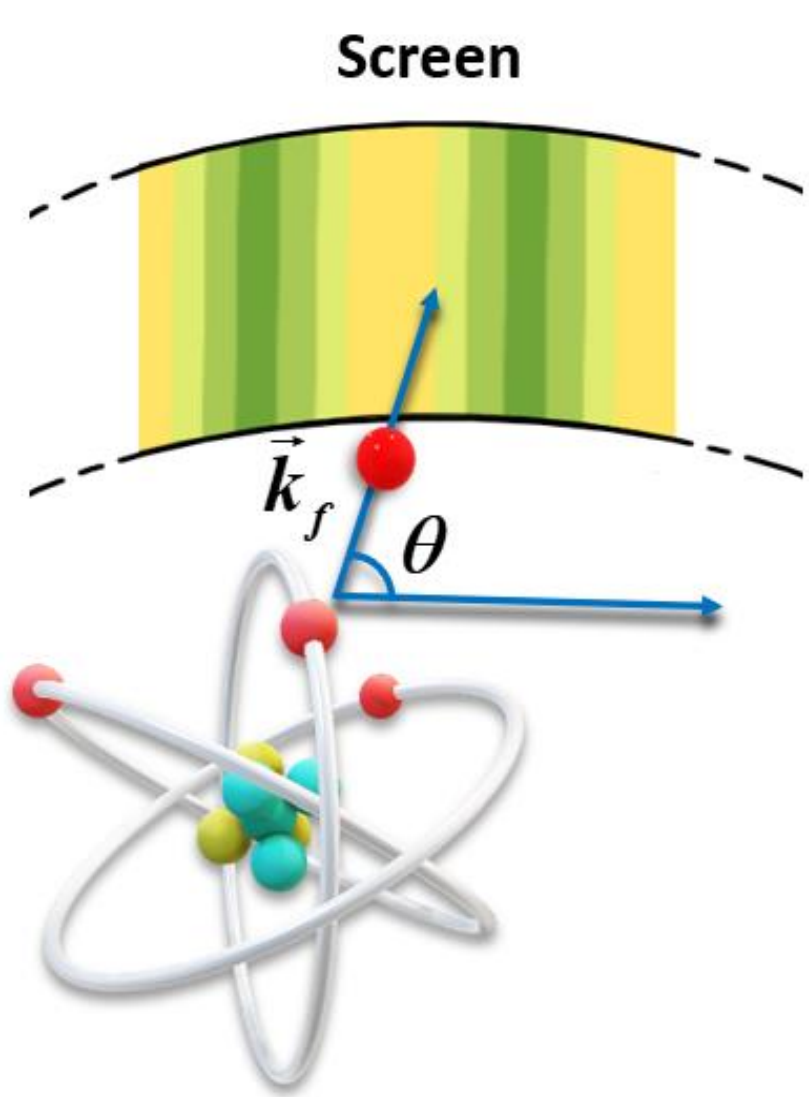
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ICAP
2024



Introduction



- Electron elastic scattering.
- Differential cross-section (DCS) measures the fraction of scattered particles in a given direction per unit solid angle [1].
- Electron density of the target atom is modelled using Multiconfiguration Dirac Fock (MCDF) method.

MCDF calculation of DCS: What is new?

- Ground state and excited state configurations of the target atom are considered. Hence a more realistic representation of the physical system.
- Different levels of correlation effect introduced:
 - ❖ A multi-configurational treatment is employed to include the initial state correlation of the scatterer.
 - ❖ Correlation potential obtained from the local density approximation (LDA).
 - ❖ The final state correlation effects are also included by writing the outgoing electron as a linear combination of different states arising from different initial states.

Methodology

- Modelling using:

Consider the example of Ca atom

1. Dirac Fock (DF) formalism [2]

$$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2$$

2. Multiconfiguration Dirac Fock (MCDF) formalism

$$1s^2 2s^2 2p^6 3s^2 3p^6 (C_1 4s^2 + C_2 3d_{3/2}^2 + C_3 3d_{5/2}^2 + C_4 4p_{1/2}^2 + C_5 4p_{3/2}^2)$$

Similar configurational combinations are considered for other atoms also.

- Target potential form:

$$V(r) = V_{static}(r) + V_{exchange} + V_{correlation} + V_{polarisation} - iW_{absorption}$$

- Dirac partial wave analysis [1].

- Initial state configuration of the scatterer: $\psi = \sum_j C_j \psi_j$

C_j - Configuration state function (CSF)

- Final scattered state DCS:

$$\frac{d\sigma}{d\Omega} = |\sum_j C_j f_j(\theta, \phi)|^2 + |\sum_j C_j g_j(\theta, \phi)|^2$$

$f_j(\theta, \phi) \rightarrow$ Direct scattering amplitude

$g_j(\theta, \phi) \rightarrow$ Spin-flip scattering amplitude

Result and discussion

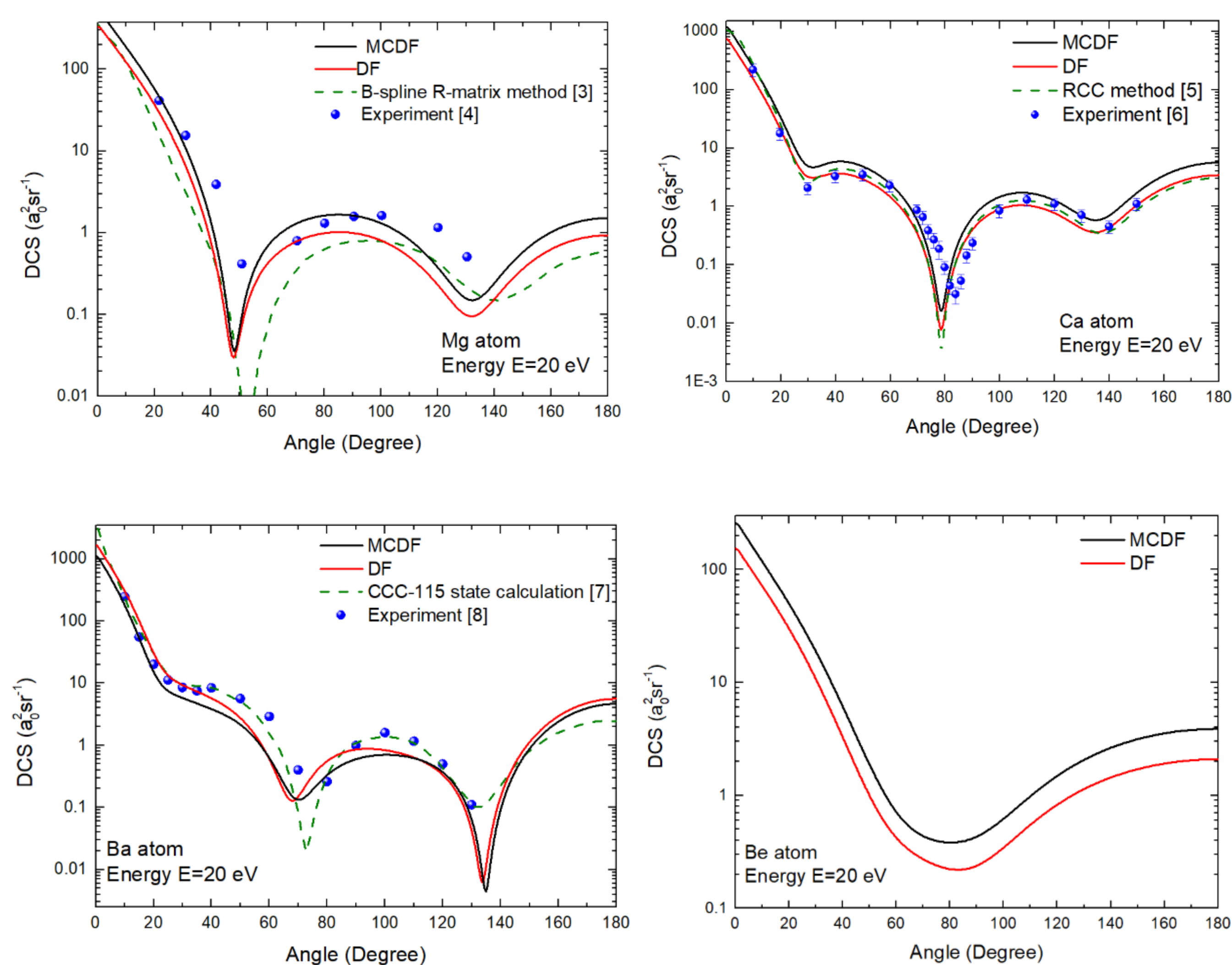


FIG. Elastic electron DCS from atoms (Mg, Ca, Ba, Be) for incident energy $E=20$ eV compared with experimental and other molecular level results.

Good agreement between MCDF results and available experimental results is noted. The obtained results also share a qualitative agreement with other molecular-level calculations.

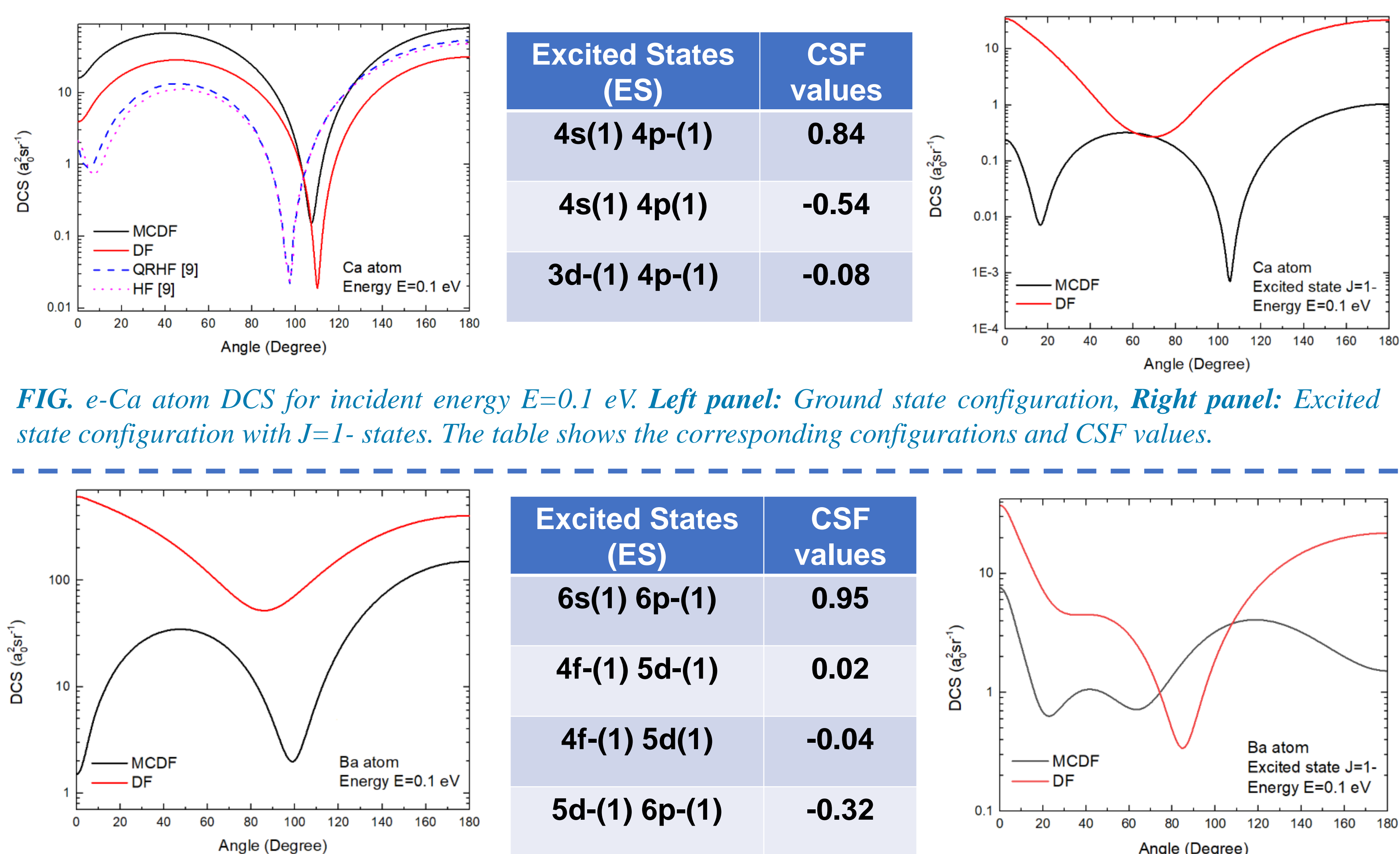


FIG. e-Ca atom DCS for incident energy $E=0.1$ eV. Left panel: Ground state configuration, Right panel: Excited state configuration with $J=1-$ states. The table shows the corresponding configurations and CSF values.

FIG. e-Ba atom DCS for incident energy $E=0.1$ eV. Left panel: Ground state configuration, Right panel: Excited state configuration with $J=1-$ states. The table shows the corresponding configurations and CSF values.

Excited state DCS computed. Results from the MCDF configuration have more oscillations in comparison with the DF results, indicating the interaction between the different excited states scattering channels of the target atom.

Conclusion

- Extension of the Dirac partial wave analysis to include multiple configurations of the target atom.
- The method could be extended to calculate the cross-section from excited state configuration.

Acknowledgement

The research is supported by DST-SERB No: CRG/2022/000191, India (J.J.) and CRG/2022/002309, India (H.R.V).

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