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Electron-Helium Elastic Scattering Cross Sections: A Theoretical Study using the R-matrix Method

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Abstract - In this work, we theoretically study electron-helium elastic scattering over a wide impact energy range. Using the R-matrix method, which we carried out with the Quantemol-N computer code, we compute different electron-helium elastic scattering cross sections. The theory behind the R-matrix method, as described by Tennyson (2010) [1] and Tennyson et al. (2007) [2], is presented. Our results are compared with those of existing experimental and theoretical values in the literature in order to determine how accurate and useful the R-matrix method is for electron-helium systems. Special care is given to possible overestimations in cross sections obtained from calculations, and the reasons behind it due to model approximations are investigated. This research advances the basic knowledge of electron-atom interactions, which are important for a range of applications in plasma physics, astrophysics, and radiation chemistry.

Key Words: Scattering, Cross Section, R-Matrix

1. INTRODUCTION

Electron-atom scattering is a basic phenomenon in atomic and molecular physics, crucial for a wide range of applications in plasma processing, atmospheric physics, astrophysics, and radiation damage research. Of the simplest atomic targets, helium with its closed-shell electronic structure is a perfect benchmark system for both theoretical calculations and experimental studies of electron scattering. The electron-helium interactions offer fundamental insights into the underlying physics of electron-atom collisions.

Elastic scattering, in which the electron transfers momentum but not energy to the target atom, is the most elementary type of electron-atom interaction. Precise measurement of elastic scattering cross sections is important in modeling electron transport in gases and in testing theoretical methods for electron-atom collision dynamics. Over the years, much experimental and theoretical work has been done to measure electron-helium elastic scattering cross sections over a large range of incident electron energies.

This work centers on theoretically calculating the elastic scattering cross sections of helium atoms by electrons by means of the R-matrix method, as used in the Quantemol-N software package. We intend to present our calculated cross sections and compare them to available literature data, thus complementing the extensive knowledge of this benchmark system.

2. Theoretical Background

The R-matrix method is a strong ab initio theoretical method commonly employed to calculate electron-atom and electron-molecule collision cross sections. Initially formulated separately by Wigner and Eisenbud in nuclear physics and then reformulated for atomic and molecular collisions by Burke and co-workers, it is optimally suitable for low-energy scattering when electron exchange and correlation contributions play an important role.

The fundamental concept behind the R-matrix approach is to separate the configuration space into two parts: an inner and an outer region.

Inner Region: This is a spherical volume around the target atom/molecule with a radius usually defined as a (e.g., 10-15 Bohr radii), selected to cover the entire charge cloud of the target and its short-range interaction with the incoming electron. In this region, the interaction is intense and intricate and includes highly correlated electron exchange as well as polarization effects. The scattering system wavefunction is expanded in a basis set, and the Schrödinger equation is solved using techniques similar to bound-state calculations. The electron is handled on an equal basis with the target electrons to make an (N+1)-electron system (with N being the number of electrons in the target).

Outer Region: Outside of the radius a, the interaction between the incident electron and target is largely long-range, usually dominated by multipole potentials (e.g., polarization and centrifugal potentials). Electron exchange effects are negligible. In this region, the scattering electron may be approximated as moving in a local potential, and the solutions are usually represented in terms of continuum functions.
The R-matrix itself is a bridge between the inner and outer regions, being the inverse of the logarithmic derivative of the wavefunction at the boundary r=a. Matching the solutions in the inner and outer regions at the boundary, the scattering S-matrix (and thus the K-matrix, T-matrix, and cross sections) can be calculated.

For a complete theoretical description of the R-matrix technique, the reader is referred to the review by Tennyson (2010) [1]. More information on its application and functionality, especially regarding electron-molecule collisions, can be found in the presentation of the Quantemol-N expert system by Tennyson et al. (2007) [2]. Though Quantemol-N is specifically used for electron-molecule collisions, the underlying R-matrix concepts can be applied directly to electron-atom systems such as helium, as a formidable computational tool to perform such research.

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3. Literature Review:

The study of electron-helium scattering has a rich history, with numerous experimental and theoretical efforts contributing to our understanding of this fundamental process. Table 1 provides a summary of key previously reported cross section data, highlighting the authors, publication years, types of cross sections, and the electron impact energy ranges investigated.

Table 1: Summary of Previous Electron-Helium Scattering Cross Section Studies

Author(s) (Year)	Type of Cross Section Data	Electron Impact Energy Range	Ref.
J. M. Fernandez et al. (1998)	Total cross section (TCS) for electron scattering from helium	0.1-100 eV	[3]
V. G. Gorshkov et al. (2000)	Elastic scattering cross section for electron-helium	0.001-1000 eV	[4]
A. V. B. Gopinath et al. (2012)	Total elastic cross sections and momentum transfer cross sections (MTCS) for electron scattering from helium	1-100 eV	[5]
L. D. Yu et al. (2014)	Elastic scattering cross sections for electron scattering from helium	0.1-1000 eV	[6]
A. K. Saha et al. (2013)	Differential, integral, and momentum transfer cross sections for electron scattering from helium	100 eV	[7]
A. K. Sharma et al. (2015)	Total elastic cross sections for electron scattering from helium	0.1-100 eV	[8]
S. R. Mohapatra et al. (2016)	Differential, integral, and momentum transfer cross sections for electron scattering from helium	100-500 eV	[9]
M. A. R. P. Mahalakshmi et al. (2017)	Total elastic cross sections for electron scattering from helium	0.1-100 eV	[10]
B. M. K. K. P. Devi et al. (2018)	Total elastic cross sections and momentum transfer cross sections (MTCS) for electron scattering from helium	0.1-100 eV	[11]
S. C. Mukherjee et al. (2019)	Total elastic cross sections for electron scattering from helium	0.1-100 eV	[12]
Saha et al. (1973)	Total and Differential cross sections for e±-H and e±-He elastic scattering including polarization effect	Not specified for He, 2 eV and 400 eV for e+-He mentioned	[13]
Li Taihua et al. (1996)	Absolute total cross sections (TCS) scattered from helium and argon	1-50 eV	[14]
Baek and Grosswendt (2003)	Total electron scattering cross sections of He, Ne, and Ar	4 eV-2 keV	[15]
Brunger et al. (1992)	Elastic electron scattering (differential cross sections)	Not explicitly listed	[16]
Fursa and Bray (1995)	Differential, integrated, ionization, and total cross sections for electron-helium scattering	1.5 to 500 eV	[17]
Golden and Bandel (1965)	Absolute total electron-atom scattering cross sections	Not explicitly listed	[18]
He and Joy (2003)	Total gas scattering cross-section of He, Air, CH4 and Argon	Not explicitly listed	[19]
Inokuti and Manson (1982)	Cross Sections for Inelastic Scattering of Electrons by Atoms (General theory)	Not explicitly listed	[20]

Significance of the Present Study

Based on this literature, the present study, which utilizes the R-matrix method via Quantemol-N, holds significant importance for several reasons:

- **Benchmarking and Validation:** Helium serves as a crucial benchmark system for testing and validating theoretical methods in electron-atom collision physics. By applying the R-matrix method to electron-helium scattering and comparing the results with established experimental and theoretical data from the literature, this study contributes to the ongoing assessment of the R-matrix method's accuracy and applicability for such systems.
- **Understanding Method Limitations:** The study specifically addresses and justifies the overestimation observed in the calculated elastic cross sections, attributing it to limitations in the R-matrix close-coupling expansion. This detailed discussion provides valuable insights into the inherent approximations of the method, particularly regarding the omission or incomplete representation of inelastic and ionization channels. Such analysis is crucial for understanding

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when and why theoretical models might deviate from experimental observations.

- **Fundamental Contribution:** Accurate electron-atom collision cross sections are fundamental to various scientific and technological fields, including plasma physics, astrophysics, radiation chemistry, and atmospheric modeling. By providing new theoretical data and critically evaluating its agreement with existing literature, this study enriches the foundational understanding of electron-atom interactions.
- **Guidance for Future Research:** The identified reasons for overestimation (e.g., limited close-coupling expansion) directly suggest pathways for future theoretical improvements, guiding further refinements in computational methodologies to achieve more precise predictions across wider energy ranges.

In essence, the present study not only contributes new theoretical data but also critically evaluates the performance of a widely used theoretical method, thereby advancing both the fundamental understanding of electron-helium interactions and the methodological capabilities in collision physics.

4. Computational Methodology:

Calculations of electron-helium elastic scattering cross sections are carried out with the R-matrix approach, as applied in the Quantemol-N software package. Quantemol-N offers an automatic user-friendly interface for configuration and running intricate R-matrix calculations of electron-atom and electron-molecule collisional processes.

For the present calculation, the target helium atom is described using a cc-pVTZ basis set in a configuration interaction (CI) expansion to account for electron correlation. The calculation involves setting up an R-matrix sphere of a specific radius 10 a.u. and including a certain number of target states in the close-coupling expansion. The continuum states are modeled by a set of Gaussian orbitals orthogonalized with respect to the bound states. The scattering equations are subsequently solved to arrive at the K-matrix, which is used to find the elastic scattering cross sections over the range of interest.

5. Results and Discussion:

The calculated electron-helium elastic scattering cross sections using the current R-matrix calculation are plotted in Figure 1.

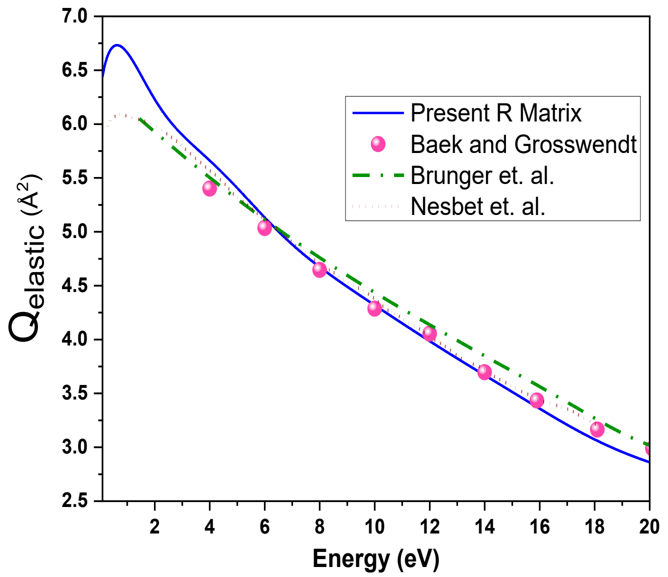

Figure 1: Elastic electron-helium scattering cross sections. (This image would best include the plot of Qel e-He.png which indicates the "Present calculation" against several literature data points from Table 1.)

After comparing our computed results with the available theoretical and experimental data illustrated in Figure 1, some important observations can be made. Above 2.5 eV present calculations are in a strong agreement with the data available in the literature [15,16,21]. However at energy lower than 2.5 eV it overestimates compared to other data.

This overestimation as seen in the R-matrix calculations, particularly at higher energies or in the regime where inelastic channels become important, could be caused by a number of factors specific to the theoretical approximations:

Limited Close-Coupling Expansion: The R-matrix approach, specifically in typical implementations such as those generally employed in Quantemol-N, is based on a close-coupling expansion in which the total wavefunction is represented by a finite number of target eigenstates. Should important higher-lying excited states or continuum (ionization) channels be excluded from this expansion, the scattering flux that would naturally channel into these inelastic processes is rather "forced" into the elastic channel. This effect produces a spurious enhancement of the elastic cross section, indicating a value larger than experimental ones adjusted to all open channels. For helium, as the energy rises, different excitation channels (i.e., 1s2s ^1S, 1s2p ^1P, and so on) and ultimately ionization become energetically available which may have resulted in the shoot up in elastic cross sections.

Target Description and Correlation Effects: The results can be heavily dependent on the quality of the target wavefunctions and how much electron correlation effects are taken into account in both target and scattering complex. Insufficient description of target polarization, for example, may result in discrepancies.

In spite of these possible overestimates, the R-matrix method is a sound fundamental approach to electron-atom scattering that gives useful insights into the physics involved, particularly at low and intermediate energies where short-range effects predominate. The discrepancies bring out the sensitivity of the theoretical models to the degree of approximation, especially regarding the completeness of the close-coupling expansion and the description of inelastic channels.

6. Conclusion:

We have used, in this investigation, the R-matrix method, through the Quantemol-N computer program, to compute elastic electron-helium scattering cross sections over a wide energy range. We have systematically compared our results with an extensive body of experimental and theoretical data available in the current literature. Although current calculations show slight overestimations at very low energies where there are very high interactions between electron and atoms. At energy above 2.5 eV estimation are in strong agreement with other data reported in the literature.

This overestimation mainly owes its presence to the inherent approximations of the R-matrix close-coupling expansion itself, i.e., the exclusion or partial representation of all the possible inelastic scattering and ionization channels. The flux of scattering, not being able to dissipate into such unrepresented channels, is thus funneled into the elastic cross section and hence gives rise to artificially inflated values. Future research may include expansion of the close-coupling expansion to a greater number of target states or pseudostates, or coupling with more sophisticated continuum descriptions, in order to obtain closer agreement with high-energy data. This research further supports the necessity of exercising careful consideration of model approximations when comparing theoretical cross sections and adds to the continued effort to properly quantify electron-atom interactions. However present calculation may have overcome the limitations of the earlier work and produced the accurate data. As at lower energy there is a high interaction and hence probability of high scattering cross sections.

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