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Benchmark Integral Cross Sections for Electron Impact Excitation of the $n = 2$ States in Helium*

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Abstract In this paper, we present integral cross sections (ICS) for electron impact excitation of the $n = 2$ levels in helium in the impact energy range of 23.5 eV to 35 eV. The ICS of each final state, 2^3S , 2^1S , 2^3P and 2^1P , has been determined by integration of the angular differential cross sections (DCS) over all of 0° to 180° , where those DCS were obtained from both our previous experiments and the extrapolation using the convergent close coupling calculation. The present experimental ICS for the optically allowed 2^1P transition state are also compared with those obtained from the BEf-scaling method. Very good agreement between the experimental and BEf-scaled 2^1P ICSs is generally found in the measured impact energy region.

Keywords: low energy electron impact, electronic excitations, helium

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1 Introduction

Inelastic cross sections for electron impact excitation of the $n = 2$ levels in helium are scientifically important from both fundamental and applied perspectives, particularly at energies in the range from the first ionization threshold to below about 35 eV. These cross sections dominate the discrete inelastic processes for both the optically allowed 2^1P transition state, as well as in near-threshold excitation for the optically forbidden 2^3P , 2^1S and 2^3S states. From the theoretical perspective, the helium system has also become a standard case to evaluate the validity of collision theory, because a three-electron system in the Coulomb field is fundamental in understanding quantum mechanical collision dynamics. This is particularly true for an appreciation of the exchange interaction and also for typical electron-correlation phenomena. From an applied perspective, knowledge of these cross sections is essential in the design of fusion reactors. This follows as helium is generated as a by-product (usually called ‘ash’) in the fusion reactor, which can then contribute as one of the important plasma-temperature loss processes in the reactor. On the occasion of the development of the ITER project, it is therefore worthwhile to provide a reliable database of helium cross sections so that these effects can be accounted for in its final design.

Recently, especially in low incident energy regime, there have been many high quality measurements of differential cross sections (DCS) focusing on excitation of the $n = 2$ levels. These include data from BRUNGER et al^[1], TRAJMAR et al^[2], CARTWRIGHT et al^[3] and RÖDER et al^[4] who employed a conventional crossed-beam approach in conjunction with a hemispherical electrostatic monochromator and analyzer. ALLAN and colleagues^[5,6] and CUBRIC et al^[7] have built magnetic angle changer devices into their spectrometers. LANGE et al^[8] and Le CLAIR et al^[9] have also measured the DCS utilizing a time-of-flight technique. Recently, we have reported benchmark DCS data for electron impact excitation of the $n = 2$ levels, including new experimental data and convergent close-coupling (CCC) calculations, at near-ionization threshold energies^[10]. In this paper, we present the corresponding experimental integral cross sections (ICS) for the 2^3S (threshold energy, $E_{th} = 19.8$ eV), 2^1S ($E_{th} = 20.6$ eV), 2^3P ($E_{th} = 20.9$ eV), and 2^1P ($E_{th} = 21.2$ eV) states. These ICS were obtained from the DCSs^[10] at near-ionization threshold energies below 35 eV. We also further test the validity of the BEf-scaling method suggested by KIM^[11], by comparing its ICS with experimental ones for the dipole allowed transition to the 2^1P state in the low energy region.

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2 Experimental procedures

To measure the inelastic differential cross sections for $n=2$ electronic state excitation of helium, a crossed beam apparatus has been employed. A detailed description on its usage is provided elsewhere^[12] and it will therefore only be briefly summarized here. Electrons from an electrostatic hemispherical monochromator intersect with an effusive helium beam at right angles, and the scattered electrons are energy-analyzed in a second hemispherical analyzer. Note that high purity helium was used throughout our measurements. Both the monochromator and the analyzer are enclosed in differentially pumped casings, respectively, to reduce the effect of background gases and to minimize any stray electric fields as well as to minimize any electron background. The incident energy of electron is calibrated against the 19.36 eV resonance of helium^[13]. With respect to the incident electron beam, the scattered electron angular range covered is from 10° to 130° , with an angular resolution of $\pm 1.5^\circ$. The cross section normalization method employs a measurement of the ratio of the inelastic to elastically scattered intensity of helium under the same experimental conditions, and the use of the known elastic differential cross sections^[14] for the particular kinematical conditions under study. Experimental errors are estimated at 15% to 20%, including components due to the uncertainty in our analyzer transmission response, an uncertainty due to errors associated with the elastic normalization cross sections and uncertainties due to any fluctuations in target density and/or incident electron beam current during the measurements. The experimental DCS have been measured at the energies of 23.5 eV, 24 eV, 25 eV, 27.5 eV, 30 eV and 35 eV for each final electronic state of the $n=2$ levels.

3 Theoretical description

The details of the CCC method for electron-helium scattering have also been given earlier by FURSA and BRAY^[15]. Briefly, an orthogonal Laguerre basis is first used to diagonalize the He^+ ion Hamiltonian to obtain negative- and positive-energy one-electron orbitals. These are then used to build up two electron configurations with one of the orbitals being the He^+ 1s orbital. This is known as the frozen-core approximation and leads to a reduction of 0.84 eV in the helium ionization energy (24.6 eV). By relaxing the frozen-core approximation we can improve the ionization energy, but at a price of generating many more states for subsequent scattering calculations. Instead, we reduce the incident energy by 0.84 eV and thereby ensure that the total energy in the CCC calculation is the same as in the experiment. As all of the helium discrete excited states are excellent frozen-core states, this approximation is adequate for our purposes.

The helium Hamiltonian is next diagonalized utilizing the built-up two-electron configurations of appropriate

symmetry to obtain the helium states to be used in the scattering calculations. By the building up, the number of helium states is (almost) twice the number of one-electron orbitals. These states are used to expand the total wavefunction which results in the close-coupling equations. The CCC formulation is in momentum space with the equations in the form of coupled Lippmann-Schwinger equations. These are solved, after partial wave expansion, typically for the first 10 to 20 partial waves, with analytical techniques ensuring the treatment of all partial waves when necessary. The solution of the coupled equations leads to the scattering amplitudes that are used to generate data for comparison with experiment.

Convergence in the scattering amplitudes needs to be established against the free parameters of the Laguerre basis. These are the basis size N_l and the exponential fall-off parameter λ_l , for orbital angular momentum $l \leq l_{\text{max}}$. Given that presently we are interested in $n=2$ excited states, setting $l_{\text{max}}=4$ is sufficient. To make the study of convergence considerably simpler, we set $\lambda_l = \lambda_0$ and $N_l = N_0 - l$. This leaves us to check convergence with just the two parameters N_0 and λ_0 . The rate of convergence for a particular experimental observable is energy dependent. In this work, we present the results in the energy range of 23.5 eV to 35 eV. Rather than finding the optimal combination of N_0 and λ_0 , at each presented energy, we carried out calculations increasing N_0 from 15 to 20 and varying λ_0 from 1.5 to 2.0 to find a single set of parameters that yields sufficiently convergent results for all of the presented cross sections at all of the energies. By taking $N_0=20$ and $\lambda_0 = 2.0$ we believe that the presented results are converged to within 5% at most scattering angles, within the frozen-core model.

4 Results and discussion

4.1 Differential cross sections

In Fig. 1(a)~(d), we present the results of 30 eV DCS from our previous experimental investigation^[10] into electron impact excitation of the $n=2$ levels in helium. The results from our corresponding CCC calculations and, where possible, data from previous experimental studies are also plotted in Fig. 1^[1,3~7,10,16,17]. This work is repeated here because in our publication^[10] we inadvertently omitted the important study from CUBRIC et al^[7]. Note that all the error bars plotted on our data in Fig. 1 represent a one standard deviation level estimate of the uncertainty on the present measurements. A very good agreement was clearly shown in general between the DCSs of our CCC calculations and all the available experimental DCS data for each final state at 30 eV. In more detail, it is clear from Fig. 1(a) that for excitation of the 2^3S state, the shapes of their angular distributions suggest important destructive and constructive interference effects between the partial waves, whereas in Fig. 1(b),

the 2^1S cross section exhibits a very deep minimum in the scattering angle range of 40° to 60° . These minima are observed in both our measurements and CCC calculations, with the experimental depth being shallower than predicted by our theory. However, this difference is simply understood in terms of the finite angular resolution ($\pm 1.5^\circ$ (FWHM)) of our spectrometer. For the 2^3P state (Fig. 1(c)), we believe that exchange will be the predominant scattering process with their angular distributions, which increase monotonically in magnitude with the scattering angle, until around 130° where they then start to again decline in magnitude, being consistent with that population mechanism. Finally, in Fig. 1(d) for the 2^1P excitation, corresponding to the dipole allowed transition, the angular distributions are forward peaked, with the degree of forward angle peaking in the cross sections increasing as the incident electron energy increases. In the cases of the other impact energies, our DCSs have shown similar behavior to those at 30 eV and all have agreed very well with the CCC calculation results^[10]. On this basis it is believed that the $n = 2$ level scattering systems in helium have been benchmarked.

Fig.1 Differential cross sections for 30 eV electron impact excitation of the $n = 2$ levels in helium, (a) 2^3S , (b) 2^1S , (c) 2^3P , and (d) 2^1P states. The present data ($\bullet$) and CCC calculated results (solid curves) are compared against the previous data from BRUNGER et al ($\circ$), ASMIS and ALLAN ($\oplus$), RÖDER et al ($+$), HALL et al (Δ), TRAJMAR ($\diamond$), CARTWRIGHT et al ($*$) and CUBRIC et al ($\times$). The estimated uncertainties on the DCS data are 15%

4.2 Integral cross sections

Integral cross sections (ICS) for each final electronic state have now been obtained at the measured impact energies of 23.5 eV, 24 eV, 25 eV, 27.5 eV, 30 eV, and 35 eV. In general, these ICS are determined by integration of the DCS over the entire range of scattering angle from 0° to 180° . In the present case, we have used our measured DCS and those obtained by an extrapolation based on the CCC calculation for the inaccessible angular ranges $\theta \leq 15^\circ$ and $130^\circ \leq \theta$. In Figs. 2(a)~(d), the current ICSs for each final state together with the previous measurements^[16~20] are shown as a function of impact energy. All of our ICSs for each final state are found to agree with the previous studies to within our experimental errors.

Fig.2 Integral cross sections for transitions to (a) 2^3S , (b) 2^1S , (c) 2^3P , and (d) 2^1P states as a function of impact energy. The term, E_{th} , corresponds to the threshold energies of each final state. The present data ($\bullet$) and CCC calculated results (solid lines) are compared against the previous data from CUBRIC et al ($\times$), PICHOU et al ($+$), HALL et al (Δ), TRAJMAR ($\diamond$), CARTWRIGHT et al ($\circ$), WESTERVELD et al ($\otimes$), and SHEMANSKY et al ($*$)

For the transition to the 2^3S and 2^1S states, the behaviors of these ICSs are very similar, namely their magnitude increases drastically from their E_{th} until about 22 eV, thereafter it decreases slowly as the impact energy increases. For the 2^3P state, the ICS has a broad maximum around 30 eV and then it decreases slowly in magnitude like the 2^3S and 2^1S states. On the other hand, for the optically allowed transition to the

2^1P state, the ICS increase smoothly from the E_{th} as the impact energy increases. Our 2^1P ICS, especially, is connected well with the data of SHEMANSKY et al [20] for near excitation threshold energies. The data embodied in Fig. 2, also clearly presents a strong support for the $n = 2$ level ICSs to be considered to be benchmarked. This is certainly to be expected given what we found at the DCS level, as described above.

4.3 Scaling law for the dipole allowed 2^1P transition

In order to discuss the dipole allowed transition to the 2^1P state in more detail, we have compared our ICS in Fig. 2(d) with the ICSs obtained from a BEf-scaling law, which was originally suggested by KIM [11]. A full description of the BEf-scaling approach for calculating ICSs with atoms and molecules can be found in Ref. [11]. The BEf-scaling method can derive ICSs of the dipole allowed electron impact transitions using the plane wave Born (PWB) approximation. In this formulation the ICS for transition to state a , σ_{ICS} , is given as

$$\sigma_a = \frac{E_0}{E_0 + B + E} \frac{f_{accr}}{f_{Born}} \sigma_{Born}.$$

Here σ_{Born} is the integral cross section calculated by the PWB approximation. The E_0 , B , and E are the impact energy of incident electron, and the binding energy and excitation energy of the target, respectively. The term, $E_0/(E_0 + B + E)$, corrects the deficiency of the PWB approximation at low E_0 without losing its validity at higher E_0 . The term of f_{accr}/f_{Born} plays the role of replacing the wavefunction used to calculate σ_{Born} with an accurate wave function, where f_{accr} and f_{Born} are the accurate dipole f -value and dipole f -value calculated from same wavefunction as used for σ_{Born} .

Fig. 3 shows the comparison between the present ICS results, including relevant previous measurements, and the scaled σ_{2p} . Given the very good agreement between our ICSs, as well as all the other available 2^1P experimental ICSs [3,7,16,17,20], and the scaled ICS from the simple PWB approximation [21], it follows that the scaling law should also be very useful to estimate ICSs, for the dipole allowed transition of the helium 2p transition, in the experimentally challenging near threshold energy region.

5 Conclusion

We have reported new experimental and CCC-calculated results of integral cross sections for electron impact excitation of the 2^3S , 2^1S , 2^3P and 2^1P levels in helium, for electrons with incident energies in the range of 23.5 eV to 35 eV. Agreement between the present results and available earlier measurements was generally good in this near threshold energy region. The present

Fig.3 Integral cross sections of the optically allowed transition to the 2^1P state in a wider energy range. The present data ($\bullet$) and present CCC calculated results (broken line) are shown together with the previous works from HALL et al (Δ), CUBRIC et al. ($\times$), CARTWRIGHT et al. ($\circ$ and $- - -$), and the others are found in Ref. [21]. The BEf-scaling results is given by the solid line in this plot

and previous integral cross sections of the dipole allowed transition to the 2^1P state were also compared with ICS obtained from the BEf-scaling law over a wider energy region. A very good agreement between the present and previous results and the scaled ICS, obtained from the simple plane wave Born approximation, was found in the energy range considered. While some small deviations do remain, the present ICS results further confirm that the $n = 2$ excitation in helium is a scattering system that can be considered to have been benchmarked.

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