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# Electron impact ionization of helium, neon and argon at intermediate energies

## Abstract

With a relatively simple distorted-wave model, in which the ejected and the scattered electrons see different residual systems depending on their energies, in this paper we show the calculation of the CPE cross sections for electron impact ionization of He, Ne and Ar. Combined with the 'maximum interference' exchange approximation, this model gives results which for Ne and Ar are in better agreement with the experiment than the other existing theoretical models.

**Keywords:** electron impact ionization, noble gases, quantum models for atomic collisions

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**Abbreviations:** CCC, convergent close coupling; BED, binary encounter dipole; CCO, coupled-channel-optical

## Introduction

Ionization of noble gases by electron impact is a process for which accurate experimental integrated cross sections are available. We shall refer in this paper to the most recent data of Rejoub et al.[1] On the theory side work is still needed for atoms heavier than helium. For helium the convergent close coupling (CCC) method[2] can produce an excellent agreement with the experiment. In the CCC method the convergence of the results is tested by including an ever increasing set of target states. These target states are obtained by diagonalizing the target Hamiltonian in an orthogonal Laguerre basis. Excellent agreement with the experiment is also obtained with the binary encounter dipole (BED) model.[3] In this approximation the continuum dipole oscillator strength is calculated from the relativistic random-phase approximation. The CCC and the BED methods were not applied to heavier targets than helium.

The distorted wave Born approximation is another method to obtain electron impact ionization cross sections for helium.[4] This is a first-order perturbation theory, which can be easily applied to other heavier targets. An elaborate calculation with this model, using distorted waves calculated for static, exchange and polarization potentials, was able to reproduce the helium experimental ionization cross sections, except in the peak range where the theoretical cross sections are slightly higher than the measurements.

For neon and argon theoretical cross sections produced by various methods are in general significantly higher than the experimental data. These methods include time-dependent close coupling calculations of Pindzola et al.[5] This paper presents cross sections for the ionization of one of the outer shell electrons of neon. The inner shell electrons are treated with pseudopotentials, while the remaining core electrons of the outer shell are handled in a configuration-average approximation. Another paper in this group is the coupled-channel-optical (CCO) model of McCarthy and Zhou.[6] CCO is a close coupling approximation which, in addition to the discrete channels, has a coupling potential that includes an *ab initio* polarization part describing the excitation of the continuum. This paper presents CCO ionization cross sections for all noble gases. The distorted-wave-R-matrix hybrid model of Bartschat and Burke[7] uses a two-state R-matrix approach in combination with a distorted-wave Born approximation. Their paper presents electron impact ionization cross sections for argon. The distorted wave Born approximation was applied by Younger[8] to the calculation of the electron impact ionization of argon. In this paper the distorted waves were obtained for potentials which accounted for the interaction between the free particles and the target nucleus and bound electrons.

A different situation exists in the case of positron impact ionization, where for all the noble gases simple distorted-wave models can produce cross sections which are in good agreement with some experiments.[9] One such model is CPE, a model which considers the full energy range of the ionization system and represents the leptons with either Coulomb or plane waves. Model CPE was introduced by Campeanu et al.[10] for positron impact ionization of helium. CPE will be discussed in detail in the next section. This paper presents CPE cross sections for electron impact ionization of He, Ne and Ar.

### The electron impact ionization

The electron impact ionization total cross section can be written as:

$$Q\left(E_i\right) = \frac{16}{\pi E_i}\int_0^{E/2} dEe\Sigma_{l_i l_e l_f}\ (2L+1)\ I\left(l_i l_e l_f\right) \quad (1)$$

where $l_i$ $l_e$ $l_f$ represent the orbital angular momentum quantum numbers of the incident, ejected and scattered electrons respectively, $E_i$ is the energy of the incident electron, $E_e$ the energy of the ejected electron, $E=E_i–I$ $E_e+E_f$ is the total energy of the scattered electrons, with $I$ the ionization energy. $I\ (l_i\ l_e\ l_f)$ can be approximated in the 'maximum interference' model [11] as:

$$I\ \left(l_i l_e l_f\right) = \left|F\right|^2 + \left|G^0\right|^2 - \left|F\right|\left|G^0\right| \quad (2)$$

where $F$ is the direct scattering amplitude and $G^0$ the singlet exchange amplitude, defined by the same expression as $F$, but with the energies of the ejected and scattered electrons interchanged.

The scattering amplitudes are obtained by first calculating the wave functions of the leptons in different channels of the ionization system. In the model CPE these wave functions of the ejected and scattered electron were calculated numerically for an electrostatic potential which depends on their energies. In model CPE the incident electron sees a neutral atom and therefore $V_i = 0$.

When the ejected electron is faster than the scattered electron (i.e. $E_e > E_f$) it sees the residual atomic ion plus the scattered electron, which we approximate to be the neutral atom. Consequently for these energies we use $V_e = 0$. We assume that the scattered electron sees only the atomic ion and therefore $V_f = -\frac{1}{r}$.

When the ejected electron is slower than the scattered electron (i.e. $E_e < E_f$) it sees only the residual He+ and we use $V_e = -\frac{1}{r}$. For these energies it is the scattered electron which sees both the residual atomic ion and the ejected electron, which we approximate to be a neutral atom $\left(i.e. V_i = 0\right)$.

We also introduce model DCPE which is different from CPE only in the representation of the channels which use plane waves (i.e. with the potential $V=0$). In DCPE we replace $V=0$ with the sum the static and polarization potentials: $V = V_{st} + V_{pol}$.

## Electron impact ionization cross sections for He, Ne and Ar

Table 1 presents our total ionization cross-sections for helium. This table shows that the DCPE data are only slightly higher than the CPE data. As the same situation was found to be true for neon and argon we shall not present the DCPE results in the graphs.

**Table 1** Electron-helium ionization cross sections (in $10^{-16}$ $cm^2$) in the CPE and DCPE models

| Energy (eV) | He(total) | |
|---|---|---|
| | CPE | CPE |
| 50 | 0.233 | 0.240 |
| 60 | 0.307 | 0.314 |
| 80 | 0.386 | 0.391 |
| 100 | 0.409 | 0.412 |
| 120 | 0.41 | 0.414 |
| 200 | 0.350 | 0.354 |
| 300 | 0.270 | 0.274 |
| 400 | 0.230 | 0.233 |
| 500 | 0.198 | 0.201 |

Figure 1 presents the comparison of our CPE results and the experimental data of Rejoub et al.[1] In addition to the CPE data Figure 1 also contains the DWE data from the paper by Campeanu et al.[4] and the coupled-channel-optical (CCO) results of McCarthy and Zhou.[6] We do not present the results of references[2] and,[3] which are in perfect agreement with the experiment.

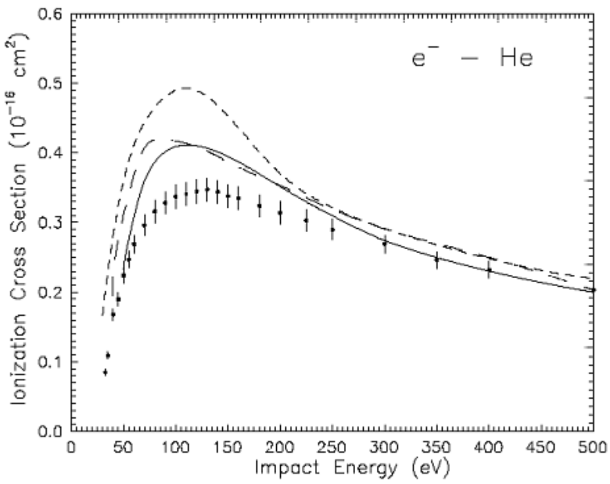


**Figure 1** Total cross-sections for electron impact ionization of He as a function of the electron impact energy.

The experimental points are from Rejoub et al.[1] The short dashed line corresponds to reference,[6] the long dashed curve to reference[4] and the solid line to model CPE.

This figure shows that the distorted wave method provides a better agreement with the experiment than the CCO method. We also found that the agreement with the experiment is quite similar for both distorted wave models in spite of the differences in their complexity. The DWE calculation of reference[4] employed in all scattering channels elaborate distortion potentials containing the static potential, polarization, and exchange. The CPE model contains by comparison very simple descriptions of the various scattering channels. In spite of these theoretical differences both models produce cross sections in good agreement with the experiment except in the peak range where they are higher than the experiment by maximum 13.8%.

Table 2 and Table 3 present total cross sections for the ionization of the two most external shells of neon and argon. For argon we also added the contribution from the 2p and 2s shells, which have an impact on the total cross sections for the 500 eV case.

**Table 2** Electron-neon ionization cross sections (in $10^{-16}$ $cm^2$) in the CPE model

| Energy (eV) | Energy (eV) | Ne(2s) | Ne(total) |
|---|---|---|---|
| 60 | 0.403 | | 0.139 |
| 80 | 0.559 | | 0.559 |
| 100 | 0.596 | 0.077 | 0.673 |
| 120 | 0.601 | 0.108 | 0.708 |
| 200 | 0.543 | 0.165 | 0.728 |
| 350 | 0.409 | 0.164 | 0.728 |
| 500 | 0.323 | 0.139 | 0.462 |

**Table 3** Electron-argon ionization cross sections (in $10^{-16}$ $cm^2$) in the CPE model

| Energy (eV) | Ar(3p) | Ar(3s) | Ar(2s+2p) | Ar(total) |
|---|---|---|---|---|
| 30 | Ar(total) | | | 1.364 |
| 40 | 1.957 | | | 1.957 |
| 60 | 2.409 | 0.251 | | 2.660 |
| 80 | 2.464 | 0.442 | | 2.906 |
| 100 | 2.385 | 0.542 | | 2.927 |
| 120 | 2.262 | 0.581 | | 2.843 |
| 200 | 1.748 | 0.546 | | 2.294 |
| 350 | 1.075 | 0.368 | | 1.443 |
| 500 | 0.711 | 0.249 | 0.15 | 1.110 |

Figure 2 and Figure 3 compare the sum of the shell ionization cross sections with the experimental data. Figure 2 shows that the time-dependent close coupling calculations of Pindzola et al.[5] are well above the experiment, while the CCO model of McCarthy and Zhou[6] agrees with the experiment for impact energies higher than 200 eV. For lower energies the CCO curve is significantly above the experiment. Our CPE model is the best agreement with the experiment. A small disagreement of maximum 8% is seen in the peak area, where CPE data are above the experiment.

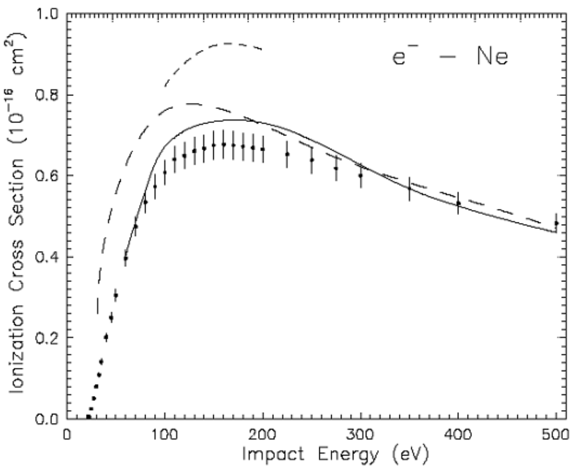


**Figure 2** Total cross-sections for electron impact ionization of Ne as a function of the electron impact energy. The experimental points are from Rejoub et al.,[1] the short dashed curve corresponds to reference,[5] the long dashed line to reference[6] and the solid line to model CPE.

Figure 3 shows that the distorted-wave-R-matrix hybrid models[7] and the distorted wave model of Younger[8] produce cross sections well above the experiment. The agreement with the experiment is better in the case of the COO method.[6] Our CPE cross sections are in the best agreement with the experiment. The disagreement in the peak area between our data and the experiment is at the level of the He agreement (i.e. CPE data are higher than the experiment by maximum 13.8%).

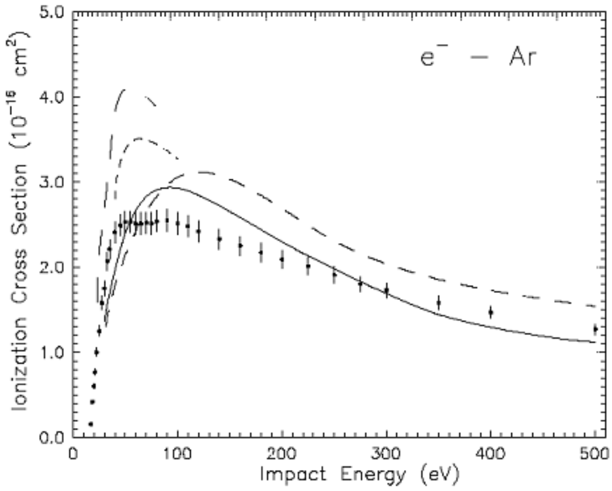


**Figure 3** Total cross-sections for electron impact ionization of Ar as a function of the electron impact energy. The experimental points are from Rejoub et al.[1] the shortest dashed curve corresponds to reference,[7] the intermediate dashed line to reference,[6] the longest dashed line to reference[8] and the solid line to model CPE.

## Conclusion

This work demonstrates that the distorted-wave model CPE can produce good agreement with experiments for electron impact ionization of He, Ne and Ar. We found that for helium CPE model produces results which have a very similar agreement with the experiment as the elaborate distorted-wave model DWE of reference.[4] For neon and argon our CPE results are in better agreement with the experiment than the other existing theoretical data. For argon the agreement with the experiment is at the level of the helium case, with the theory being above the experiment in the peak range, while for neon the agreement of CPE with the experiment is better that in the helium and argon cases. We conclude that relatively simple distorted-wave models of electron impact ionization of He, Ne and Ar can achieve the same level of success as in the positron impact case if the post-collision interactions are correctly represented.

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## Conflicts of interest

The author declares that there is no conflict of interest.

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