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Electron Impact Ionization of Krypton at Intermediate Energies

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Abstract

The distorted-wave approach is applied to electron impact single ionization of krypton. We find that our models CPE4 and DW2 give results which are in fair agreement with the experiments. Both models contain a final state representation which includes the electrostatic repulsion between the ejected electron and the scattered electron.

Keywords: total cross sections for the ionization of atoms through electron impact; distorted-wave approximation

1. Introduction

Electron impact single ionization of noble gas atoms is one of the most important testing grounds for theoretical models. This is because a large number of experiments are available and because ionization processes play an important role in many areas of research, such as plasma physics or astrophysics.

Most of this research concentrated on electron impact single ionization of light noble gas atoms: He, Ne and Ar. We have found that for these atoms the model CPE4 produces good agreement with the experimental data [1]. CPE4 uses plane waves for the incident and scattered electron and a Coulomb wave function for the ejected electron. The Coulomb wave function was calculated with a potential that includes the electrostatic repulsion between the ejected and scattered electrons.

In this paper we want to study the electron impact single ionization of krypton, a heavy noble gas atom. There are several experiments measuring total ionization cross sections for electron impact ionization of krypton [2–4]. Their results mostly agree with each other.

On the theory side we found five papers which calculate the total ionization cross section for electron impact ionization of krypton. The theoretical paper by Bartlett and Stelbovics [5] used a Born approximation in which the ejected electron Coulomb wave function is orthogonalized to all occupied atomic orbitals (BCO). The paper by McCarthy and Zhou [6] used a coupled-channel-optical (CCO) model. This model is a numerically simple way of including the continuum in a coupled-channel calculation. Loch et al. [7] used a configuration-average distorted waves (CADW) model. In this method contributions to the cross sections are included from both direct ionization and excitation autoionization. The papers by Jha et al. [8] and Tsipinyuk et al. [9] used the binary encounter approximation (BEA). BEA is a semi-classical method which treats the collision as an isolated, two-body interaction between the incident projectile and a single target electron.

Most of these models gave ionization cross sections which are for all electron impact energies above the experimental data. The lowest theoretical cross sections were obtained

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in the BEA paper [8]. The CADW [7] results were the highest. At an impact energy of 90 eV the peak calculated with CADW was about double the size of the experimental data.

In the present work we apply for the ionization of krypton two variants of the Distorted-Wave Born approximation (DWBA) and the CPE4 Born approximation, which was successful for other noble gases. We compare our results with other theories and with the experimental data.

2. Theory

Within the Distorted-Wave Born approximation the wavefunctions of the incident projectile and of the emergent particles are expanded into the partial wave series. The total cross section for the single ionization of krypton is obtained as a sum over the partial waves and an integral over the energy of the ejected electron:

$$Q(E_i) = \frac{16}{\pi E_i} \int_0^{E/2} dE_e \sum_{lilelf} (2L+1) I(l_i l_e l_f), \tag{1}$$

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, and E is the total energy of the ejected and scattered electrons: $E = E_i - I = E_e + E_f$, where I is the ionization energy. Equation (1) also contains L, the total orbital angular momentum quantum number, given by: $L = l_i + l_b$, where l_b is the orbital quantum number of the bound electron to be ionized.

In the "maximum interference" approximation [10] I (l_i l_e l_f) can be written as:

$$I(l_i l_e l_f) = |t_d|^2 + |t_e|^2 - |t_d||t_e|, \tag{2}$$

where the singlet exchange amplitude t_e is defined by the same expression as the direct scattering amplitude t_d, but with the ejected and scattered electrons interchanged:

$$\begin{aligned} t_e &= \langle \phi_e(\mathbf{r}_1)\phi_f(\mathbf{r}_2)|V(r_{12})|\phi_i(\mathbf{r}_1)\phi_b(\mathbf{r}_2)\rangle, \\ t_d &= \langle \phi_f(\mathbf{r}_1)\phi_e(\mathbf{r}_2)|V(r_{12})|\phi_i(\mathbf{r}_1)\phi_b(\mathbf{r}_2)\rangle \end{aligned} \tag{3}$$

In Equation (3) ϕ_b, ϕ_i, ϕ_e and ϕ_f stand for the wavefunctions of the bound, incoming, ejected and scattered electron, respectively, while $V(r_{12})$ is the Coulomb interaction between the two active electrons. In the calculation of the amplitudes, we used plane waves and distorted waves based on the following assumptions.

The CPE4 model is a Born approximation in which both the incident electron and the scattered electron are represented with plane waves. In this model the ejected electron "sees" the positive charge of the Kr^+ ion and the negative charge of the scattered electron. The Coulomb wave function representing the ejected electron is calculated with:

$$V_e = -\frac{1 - E_e/E_{ef}}{r}, \tag{4}$$

where E_{ef} is given by

$$E_{ef} = E_e + E_f - 2(E_e E_f)^{1/2}. \tag{5}$$

In the distorted-wave models DW1 and DW2 the function ϕ_i is calculated in the field of the potential

$$V_i = V_{static} + V_{polarization}. \tag{6}$$

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We used the Hartree–Fock approximation in calculations of the krypton bound states, and of the potentials V_{static} and $V_{polarization}$.

In both models DW1 and DW2 the ejected electron function ϕ_e is calculated in the field of the potential V_e given by Equation (4). The difference between DW1 and DW2 is in the calculation of the function ϕ_f describing the fast scattered electron. In model DW1 this distorted wave is calculated using a potential V_f given by Equation (6), while in model DW2 the function ϕ_f was calculated using the potential V_f given by Equation (4).

3. Results and Discussion

Table 1 and Figure 1 present our CPE4, DW1 and DW2 total ionization cross-sections for electron impact ionization of krypton. Our theoretical results include contributions from the ionization of 4p, 4s orbitals. The number of partial waves used in the description of the electrons increased with the impact energies. For 400 eV we used 20 partial waves for the ejected electrons and 40 partial waves for the incident and scattered electrons.

In addition to our theoretical results Figure 1 also included two sets of experimental data [2,3] and the BCO [5] and BEA [8] theoretical results. We did not show the theoretical results of model CCO [6] and CADW [7], which are about equal or higher than the BCO results.

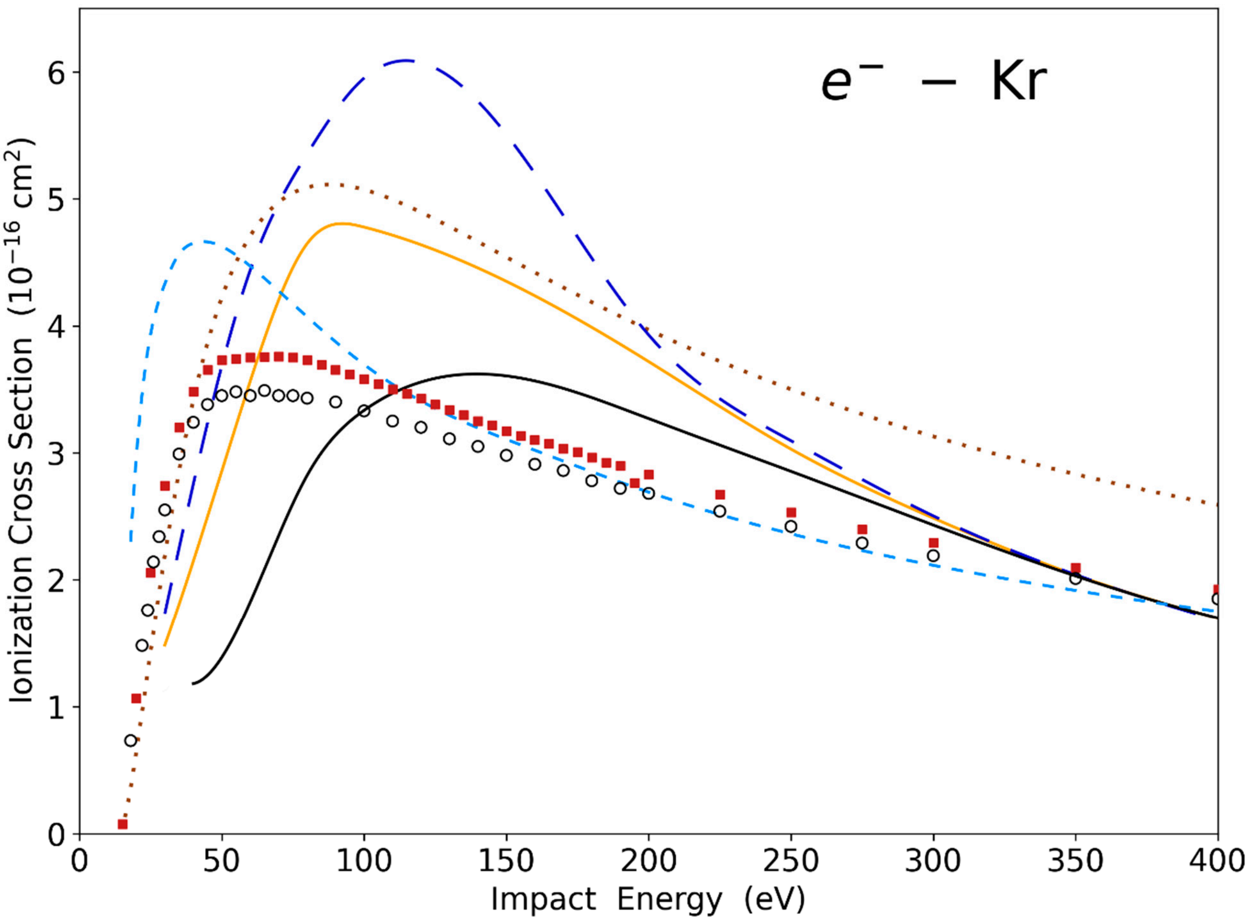

Figure 1. Total cross-sections for electron impact ionization of krypton as a function of the electron impact energy. The experimental points are from Krishnakumar et al. [2] (red squares) and Rejoub et al. [3] (full circles). The solid yellow curve corresponds to model CPE4, the long dashed blue curve to model DW1, the solid black curve to model DW2, the dotted curve to model BCO [5] and the short dashed blue curve to BEA [8].

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All theoretical models except our model DW2 and model BEA [8] overestimate the ionization cross sections for impact energies around 100 eV. Our model DW2 and model BEA [8] give results which are the closest to the experimental data, but the shape of the two curves is very different. BEA has a large peak at 40 eV impact energy, while the maximum for the DW2 curve is at 150 eV. This is a consequence of the different consideration of the post collision interactions.

Table 1. CPE4, DW1 and DW2 ionization cross-sections for electron impact ionization of the 4p and 4s orbitals of krypton. The results are in 10^{-16} cm^2 units.

Energy (eV)	CPE4			DW1			DW2		
	4p	4s	Total	4p	4s	Total	4p	4s	Total
30	1.483	-	1.483	1.733	-	1.733	0.754	-	0.754
40	2.145	-	2.145	2.752	-	2.752	1.180	-	1.180
60	3.268	0.295	3.563	4.016	0.421	4.437	1.534	0.288	1.822
80	3.806	0.841	4.647	4.473	0.880	5.353	2.346	0.476	2.822
100	3.922	0.855	4.777	4.716	1.234	5.950	2.617	0.717	3.334
150	3.359	1.038	4.497	3.843	1.268	5.111	2.731	0.809	3.540
200	2.802	0.916	3.718	2.952	0.976	3.928	2.469	0.800	3.269
250	2.262	0.767	3.029	2.312	0.783	3.095	2.138	0.716	2.854
300	1.850	0.636	2.486	1.860	0.643	2.503	1.820	0.611	2.431
350	1.513	0.525	2.038	1.508	0.532	2.040	1.520	0.510	2.030
400	1.258	0.438	1.696	1.237	0.445	1.682	1.271	0.426	1.697

Our CPE4 model results agree with the BCO model results. This agreement was expected as both models are Born approximations with an ejected electron Coulomb wave function. The difference is that in the case of the BCO model the Coulomb wave function was orthogonalized to all occupied atomic orbitals, while in our CPE4 model the Coulomb wave function was calculated after the inclusion of the repulsion between the slow ejected electron and the fast scattered electrons.

Our DW2 model produces fair results for impact energies over 100 eV, but fails to agree with the experiments at impact energies below 80eV. In this model both the ejected electron and the scattered electron are represented with Coulomb wave functions calculated after the inclusion of their repulsion. For impact energies over 100 eV DW2 results agree best with the semi-classical calculations of BEA [8].

Our DW1 model produces results which for impact energies below 200 eV are the highest in Figure 1. This model does not contain the electrostatic repulsion between the ejected electron and the scattered electron.

4. Conclusions

This work shows that for krypton, one of the heaviest noble gases, our models CPE4 and DW2 can produce fair agreement with the total ionization cross section measurements, when combined with the ‘maximum interference’ exchange approximation. Both models contain a final state representation which includes the electrostatic repulsion between the ejected electron and the scattered electron. In the case of model CPE4 this repulsion is applied only to the ejected electron, while in the model DW2 it is applied to both outgoing electrons. The DW2 model produces a peak which has the magnitude of the experimental peak, but at higher impact energy.

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Abbreviations

The following abbreviations are used in this manuscript:

CPE4, DW1, DW2	Distorted-Wave Born approximation
CCO	Coupled-channel-optical model
BCO	Born approximation using an ejected electron Coulomb wave function orthogonalized to all occupied atomic orbitals
CADW	Configuration-average distorted waves method
BEA	Binary encounter approximation

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