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Total cross sections for \((e^{-}\text{He})\) ionization

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Résumé. — On calcule les sections efficaces totales d’ionisation par impact électronique dans le domaine d’énergie 40-150 eV et dans le modèle de l’onde déformée, où l’on utilise des ondes déformées pour les électrons incidents, diffusés et éjectés. Nos résultats sont comparés aux résultats expérimentaux ainsi qu’aux autres prédictions théoriques.

Abstract. — Total cross sections for electron impact ionization have been calculated in the energy range 40-150 eV in a distorted wave model which employs distorted waves for the incident, scattered and ejected electrons. The present results are compared with experimental results and other theoretical predictions.

1. Introduction.

Ionization of helium atom by electron impact is a common process in natural plasmas. In laboratory plasmas it is particularly relevant to controlled thermonuclear fusion devices because helium is produced as a result of D-T fusion reaction. Helium is also the simplest terrestrial gas and is therefore a natural candidate for use as standard atomic collision measurements. Even also from the theoretical point of view after atomic hydrogen it is an ideal system for the study of the electron impact ionization because of the availability of accurate wave function and absence of inner shell effects.

There exists a number of experimental results for the total cross section (TCS) for electron impact ionization of helium. Recently Shah et al. [1] have measured the TCS for \((e^{-}\text{He})\) ionization using a pulsed crossed beam technique. Their results are in very good agreement with the experimental results of Montauge et al. [2]. On the theoretical side most of the recent calculations on \((e^{-}\text{He})\) ionization have been directed towards obtaining the triple and double differential cross sections [3]. Bell and Kingston [4] Economides and McDowell [5] and Sloan [6] have used the first Born approximation (FBA) to obtain the TCS for \((e^{-}\text{He})\) ionizations. But below an incident energy of 400 eV the FBA results overestimate the experimental results. Recent calculations by Bartchat and Burke [7] based on the use of the \(R\)-matrix
method provide cross sections larger than the measured values. The results obtained by Peach [8] by using the Ochkur approximation are in fair agreement with the experimental values whereas the Born-Exchange (BE) results of Peach [8] rather underestimate the measured values. The first distorted wave calculations for TCS of (e-He) ionization were performed by Bransden et al. [9] but their results overestimate the experimental results below an incident energy of 250 eV. Recently Campeanu et al. [10] have carried out an elaborate and consistent distorted wave calculation for TCS of (e-He) ionization. Their results in the model DWE are in very good agreement with the measured values above the incident energy of 150 eV but below 150 eV there is some divergence between their results and the measured values, the measured values being lower.

In the present paper we plan to calculate the TCS for (e-He) ionization in the energy range 40-150 eV. Campeanu et al. [10] have employed a full screening model. But in the low energy region (40-150 eV) under consideration the system gets ionized before the scattered (faster) electron can leave and therefore this electron like the ejected (slower) electron sees the final state of the target [11]. So we have assumed that both the outgoing electrons move in the field of the residual He+ nucleus. We have also taken into account the effects of the final channel and target distortions which have been found to be important in electron-atom scattering [12, 13].

2. Theory.

The TCS for the ionization of a helium atom by an unpolarized beam of electrons is given in terms of singlet/triplet direct and exchange scattering amplitudes by

\[ Q = \frac{1}{2 \pi^2} \int \int \frac{k_f}{k_i} \left[ |f^0|^2 - |g^0|^2 + 3 |g^1|^2 \right] \, d\vec{k}_f \, d\vec{k}_e \quad (2.1) \]

where \(k_i\) is the momentum of the incident electron and \(k_f\) and \(k_e\) are the momenta of the scattered (faster) and the ejected (slower) electrons respectively. The two outgoing electrons obey the energy conservation relation

\[ E_i = E_f + E_e + E_t \quad (2.2) \]

where \(E_i, E_f\) and \(E_e\) are respectively the energies of the incident, scattered and ejected electrons. \(E_t\) is the energy for the single ionization of helium. \(f^0\) and \(f^1\) are respectively the singlet and triplet direct scattering amplitudes and \(g^1\) is the triplet exchange scattering amplitude.

Following Geltman [14] we can write

\[ f^S = \frac{1}{2 \pi} \left( \chi_{k_f}(z_f, \vec{r}_f) \, \psi_f^S(\vec{r}_2, \vec{r}_3) \right) \left( \frac{1}{r_{12}} + \frac{1}{r_{13}} \right) \psi_i(\vec{r}_1, \vec{r}_2, \vec{r}_3) \quad (2.3) \]

\[ g^S = \frac{1}{2 \pi} \left( \chi_{k_f}(z_f, \vec{r}_f) \, \psi_f^S(\vec{r}_2, \vec{r}_3) \right) \left( \frac{1}{r_{12}} + \frac{1}{r_{13}} \right) \psi_i(\vec{r}_1, \vec{r}_2, \vec{r}_3) \quad (2.4) \]

where \(S = 0\) and \(S = 1\) stand respectively for the singlet and triplet scattering amplitudes. The subscript 1 refers to the incident electron and 2 and 3 to the helium electrons.

\(\chi_{k_f}(z_f, \vec{r}_f)\) is the wave function of the scattered electron. \(z_f\) is the effective charge as seen by the scattered electron. As we have already mentioned in the scattered electron moves in the field of the residual He+ nucleus so that \(z_f = 1\).
\( \psi_i(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) \) is the wave function of the initial state of the electron-helium system. Taking into account the effect of the target distortion it can be written as [15]

\[
\psi_i(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) = F(\mathbf{r}_1)(\mu(\mathbf{r}_2) \mu(\mathbf{r}_3) + \chi(\mathbf{r}_1, \mathbf{r}_2) \mu(\mathbf{r}_3) + \chi(\mathbf{r}_1, \mathbf{r}_3) \mu(\mathbf{r}_2))
\] (2.5)

where \( F(\mathbf{r}_1) \) is the wave function of the incident electron.

\( \chi(\mathbf{r}_1, \mathbf{r}_2) \) is the dipole component of the distorted part of the target wave function. It is given by [15]

\[
\chi(\mathbf{r}_1, \mathbf{r}_2) = - \pi^{-1/2} \frac{t(\mathbf{r}_1, \mathbf{r}_2)}{r_2} \frac{\mu_{\text{is}-p}(\mathbf{r}_2)}{r_1} \cos(\hat{r}_1 \cdot \hat{r}_2)
\]

where

\[
t(\mathbf{r}_1, \mathbf{r}_2) = \begin{cases} 1 & r_1 > r_2 \\ 0 & r_1 < r_2 \end{cases}
\]

and

\[
\mu_{\text{is}-p}(\mathbf{r}) = z_p^{1/2} \left( \frac{1}{2} z_p r^3 + r^2 \right) \exp(-z_p r)
\]

with

\[ z_p = 1.598 \, . \]

We have ignored the target distortion in the calculation of the exchange contribution to the ionization amplitude. The exchange has been introduced as if the atomic charge cloud were not distorted whereas target distortion is included as if exchange did not take place. Since the distortion of the atomic charge cloud is negligible at small distances, where exchange is the most important [16] this choice is not expected to effect the results significantly. \( \Phi_0(\mathbf{r}_2, \mathbf{r}_3) \) is the helium ground state wave function. We have used for it the analytic Hartree-Fock (HF) wave function of Byron and Joachain [17]

\[
\Phi_0(\mathbf{r}_2, \mathbf{r}_3) = \mu(\mathbf{r}_2) \mu(\mathbf{r}_3)
\]

with

\[
\begin{align*}
\mu(\mathbf{r}) &= R_4(\mathbf{r}) Y_{00}(\hat{r}) \\
R_{4s}(\mathbf{r}) &= N [\exp(-\alpha r) + \delta \exp(-\beta r)]
\end{align*}
\]

where

\[ N = 2.6049754 \, , \quad \alpha = 1.41 \, , \quad \beta = 2.61 \, , \quad \delta = 0.799 \, . \]

\( \psi_f^s(\mathbf{r}_2, \mathbf{r}_3) \) represents the final state of the helium subsystem. Following Phillips and McDowell [18] we have taken it as

\[
\psi_f^s(\mathbf{r}_2, \mathbf{r}_3) = \frac{1}{\sqrt{2}} \left[ \chi_{k_s}(z_e, \mathbf{r}_2) V(\mathbf{r}_3) + (-1)^s \chi_{k_s}(z_e, \mathbf{r}_3) V(\mathbf{r}_2) \right]
\]

where \( V(\mathbf{r}) \) is the wave function of the residual \( \text{He}^+ \) ion

\[
V(\mathbf{r}) = \left( \frac{8}{\pi} \right)^{1/2} \exp(-2 r)
\]

\( \chi_{k_s}(z_e, \mathbf{r}) \) is the wave function of the ejected electron. \( z_e \) is the effective charge as seen by the slower electron.
As already stated we have taken $z_e = 1$. It is to be noted the choice of the wave function of the helium subsystem in the singlet state is not orthogonal to $\Phi_0(r_2, r_3)$. We have orthogonalised the final state wave function in the singlet state by replacing $\chi_{k_e}(z_e, r)$ in equation (2.11) by

$$\tilde{\chi}_{k_e}(z_e, r) = \chi_{k_e}(z_e, r) - \mu(r) \left( \int \chi_{k_e}^*(z_e, r') \times \mu(r') \, dr' \right). \tag{2.13}$$

The wave function $F(r_1)$ of the incident electron is decomposed into partial waves as [15]

$$F(r_1) = k_i^{-1/2} \sum_{\ell_i = 0}^\infty (2\ell_i + 1) i^{\ell_i} \exp(i\delta_{\ell_i}) \frac{\mu_{\ell_i}(k_i, r_1)}{r_1} \times P_{\ell_i}(\cos(k_i \vec{r}_1)) \tag{2.14}$$

where $\ell_i$ is the orbital angular momentum quantum number of the incident electron. The radial part $\mu_{\ell_i}(k_i, r_1)$ of $F(r_1)$ satisfies the integro differential equation

$$\left( \frac{d^2}{dr_1^2} + \frac{\ell_i(\ell_i + 1)}{r_1^2} - 2 V_{ls}(r_1) - 2 \frac{2}{2\ell_i + 1} \right) \times \mu_{\ell_i}(k_i, r_1) = X_{\ell_i}(r_1) r_1 R_{ls}(r_1) \tag{2.15}$$

with

$$X_{\ell_i}(r_1) = (\epsilon_{ls} - k_i^2) \delta_{\ell_i} \int_0^\infty r_2 R_{ls}(r_2) \mu_{\ell_i}(k_i, r_2) \, dr_2 - \frac{2}{2\ell_i + 1} \times \int_0^\infty r_2 R_{ls}(r_2) \mu_{\ell_i}(k_i, r_2) r_{\ell_i}(r_1, r_2) \, dr_2 \tag{2.16}$$

and

$$r_{\ell_i}(r, r') = \frac{r_{\ell_i}^*}{r_{\ell_i} + 1}. \tag{2.17}$$

Equation (2.15) is to be solved subject to the usual boundary conditions,

$$\mu_{\ell_i}(k_i, 0) = 0, \quad \mu_{\ell_i}(k_i, r) \bigg|_{r = \infty} = k_i^{-1/2} \sin \left( k_i r - \frac{1}{2} \ell_i \pi + \delta_{\ell_i} \right) \tag{2.18}$$

$\delta_{\ell_i}$ is the phase shift. The polarization induced by the incoming electron is only taken into account by means of the direct polarization potential $V_{pol}(r)$ so that (2.15) produces elastic scattering solutions in the adiabatic exchange approximation, the effect of exchange polarization terms having been neglected. This is consistent with the fact that in calculating the exchange amplitude we have not considered the effect of target distortion. The direct static potential $V_{ls}(r)$ is given by

$$V_{ls}(r) = -\frac{2}{r} + \left( \mu_{ls}(t) \right| \frac{2}{|r - t|} \left| \mu_{ls}(t) \right). \tag{2.19}$$

and $V_{pol}(r)$ by

$$V_{pol}(r) = \left( \mu_{ls}(t) \right| \frac{2}{|r - t|} \left| \chi(r, t) \right). \tag{2.20}$$
We have decomposed \( \chi_{k,\lambda}(z, r) \) \( (\lambda = f \text{ or } e) \) into partial waves as

\[
\chi_{k,\lambda}(z, r) = \frac{4 \pi}{k} \sum_{l=0}^{\infty} \sum_{m=-l}^{l} l^2 \sum_{m_1=-l}^{l} G_{\ell_1}(k, z, r) \frac{Y_{\ell_1} m_1(\ell)}{r} Y_{\ell_2}^{m_2}(\ell) \exp(-i \eta_{\ell_1}) \quad (2.21)
\]

where \( \eta_{\ell_1} \) is the corresponding phase shift. \( \ell_f \) and \( \ell_e \) are respectively the orbital angular momentum-quantum numbers of the scattered and ejected electrons. The radial wave functions \( G_{\ell_1}(k, z, r) \) for both the outgoing electrons are the exchange polarization functions for the scattering of electrons by He\(^+\) ion (Sloan [19]).

### 3. Results and discussions.

The major trouble in the evaluation of scattering amplitudes \( f^S \) and \( g^S \) \( (S = 0, 1) \) is encountered in the evaluation of radial integrals occurring in them. The number of partial waves required to obtain convergence increases with energy resulting in severe cancellation in the sums over the angular momenta. We have evaluated the radial integrals upto a radial distance of 80 a.u. using 16 point Gauss-Legendre Quadrature by partitioning the entire integral into a number of integrals (Sil [20]). The radial parts of the wave functions of the incident electron and two outgoing electrons have been obtained by solving the corresponding integrodifferential equations by Numerov method (Sloan [19]) upto a radial distance of \( r = 30 \) a.u. with a step size of 0.01 a.u. For \( r > 30 \) a.u. the radial wave functions have been replaced by their well-known asymptotic forms (McDowell et al. [21]). The integral over \( k_\alpha \) in the expression for \( Q \) has been carried out by using 8 point Gauss-Legendre Quadrature. Special attention has been given on the convergence of \( Q \) with respect to the angular momentum quantum number \( \ell_\alpha \), \( \ell_e \) and \( \ell_f \). The maximum value of \( \ell_e \) has been taken as 5. For \( E_i = 40 \) eV the maximum value \( (\ell_\alpha)_{\text{max}} \) of \( \ell_\alpha \) is taken as 10 whereas for \( E_i = 150 \) eV \( (\ell_\alpha)_{\text{max}} = 20 \). \( \ell_f \) has been obtained from the triangle rule involving \( \ell_\alpha \), \( \ell_e \) and \( \ell_f \). It has been observed that for a particular value of \( \ell_\alpha \) and \( \ell_f \) contributions to \( Q \) for \( \ell_e > 5 \) correspond nearly to the terms of a geometric series. Therefore the contributions of partial waves \( \ell_e > 5 \) are approximated by the series. We have noted that at the lowest energy considered (40 eV) the error incurred due to this approximation is less than 1%.

Table I presents the total cross section \( Q \) for \( (e^-\text{He}) \) ionization calculated by using the present method together with the FBA results of Bell and Kingston [4] and DWE results of Campeanu et al. [10]. In figure 1 we have plotted the present results together with the FBA [4] and DWE results [10] and the experimental results of Shah et al. [1]. It is evident from figure 1 that although the present method provides improved agreement between the

### Table I. — **Total cross sections (in units of \( \pi a_0^2 \)) for \( (e^-\text{He}) \) ionization.**

<table>
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<td>0.4491</td>
</tr>
<tr>
<td>120</td>
<td>0.6050</td>
<td>0.4648</td>
<td>0.4393</td>
</tr>
<tr>
<td>150</td>
<td>0.5529</td>
<td>0.4408</td>
<td>0.4127</td>
</tr>
</tbody>
</table>
Fig. 1. — Total cross section ($Q$) for ($e^-$-He) ionization (in units of $\pi a_0^2$). A: FBA [4]; B: DWE [10]; C: Present results; I: Experiment [1].

theoretical results and the measured values there is still some discrepancy between them. The situation is somewhat similar to the electron impact ionization of atomic hydrogen [22]. Further improvement may await the development of methods which allow for correct asymptotic form of the final state wave function as done by Brauner et al. [23, 24] who have derived an exact form of the three-body Coulomb wave function in the asymptotic region for the electron impact ionization of atomic hydrogen by using a modification of the method of Pluvinage [25, 26].

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