Electron Impact Ionisation of the Ground State of He⁺

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Abstract

Electron impact ionisation of the ground state of He^+ is studied by using the distorted wave polarised orbital (DWPO) method in the energy range $61 \cdot 2 - 272 \cdot 0$ eV. The present results for the total cross section are in good agreement with the measured values.

1. Introduction

Cross sections for electron impact ionisation of atoms and ions at incident electron energies up to about five times the threshold value are urgently required for the study of laboratory and astrophysical plasmas. The theory of electron impact ionisation of positive ions has been reviewed by Jakubowicz and Moores (1980), Peterkop (1977), Dolder and Peart (1976) and Rudge (1968). The total cross section (TCS) for electron impact ionisation of He⁺(1s) has been measured by different workers. Dolder et al. (1961) measured the e⁻-He⁺(1s) total ionisation cross section using the crossed beam technique in the energy range from threshold (54.4 eV) to 1000 eV. Peart et al. (1969) used the same technique and extended the measurements up to 10000 eV. Defrance et al. (1981) used a new technique to measure e⁻-He⁺ ionisation cross sections in the energy range 55 to 74 eV. All these measurements diverge by an amount which is within the errors assigned in the experiments. Theoretically, Rudge and Schwartz (1966) studied the problem using Coulomb Born no exchange (CBOX) and Coulomb Born exchange (CBX) approximations and found their results to be in very good agreement with the measured values of Dolder et al. (1961). McDowell et al. (1974, 1975) have employed a distorted wave polarised orbital (DWPO) method to study the electron impact excitation of He⁺. In the present paper we have applied the DWPO method of McDowell et al. (1974, 1975) to calculate the TCS for e⁻-He⁺(1s) ionisation in the energy range $61 \cdot 2 - 272 \cdot 0 \text{ eV}$.

2. Theory

The TCS for the electron impact ionisation of He^+ in singlet and triplet modes is given by (Geltman 1969)

$$Q_{\rm ion}^{\pm} = \int \mathrm{d}\hat{k}_{\rm f} \,\mathrm{d}k_{\rm e}(k_{\rm f}/k_{\rm i}) |f_{\rm ion}^{\pm}(k_{\rm f},k_{\rm e})|^2, \qquad (1)$$

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where the superscripts (\pm) stand for singlet and triplet spin states, and k_i , k_f and k_e are the momenta of the incident, scattered and ejected electrons respectively. The TCS for an unpolarised beam of electrons is given by

$$Q_{\rm ion} = 0.25 Q_{\rm ion}^+ + 0.75 Q_{\rm ion}^-.$$
 (2)

Let r_1 and r_2 be the position vectors of the incident and target electrons with respect to the nucleus, which is assumed to be infinitely heavy. We can write the total Hamiltonian (in atomic units) as

$$H = -\frac{1}{2}\nabla_{1}^{2} - \frac{1}{2}\nabla_{2}^{2} - \frac{Z}{r_{1}} - \frac{Z}{r_{2}} + \frac{1}{r_{12}},$$

= $H_{\rm f} + V_{\rm f},$ (3)

with

$$H_{\rm f} = -\frac{1}{2}\nabla_1^2 - \frac{1}{2}\nabla_2^2 - \frac{Z}{r_2} - \frac{Z_{\rm f}}{r_1}; \quad z_{\rm f} = Z - 1, \qquad (4)$$

$$V_{\rm f} = -\frac{1}{r_{\rm l}} + \frac{1}{r_{\rm l2}},\tag{5}$$

in the direct channel. Here Z is the charge of the target nucleus, and for He⁺ Z = 2.

The final unperturbed state of the total system is then

$$\psi_{\mathbf{f}}(\mathbf{r}_{1},\mathbf{r}_{2}) = \chi_{k_{\mathbf{e}}}(z_{\mathbf{f}},\mathbf{r}_{1})\chi_{k_{\mathbf{e}}}(z_{\mathbf{e}},\mathbf{r}_{2}), \qquad (6)$$

where $\chi_{k_f}(z_f, r_1)$ and $\chi_{k_e}(z_e, r_2)$ are the outgoing Coulomb waves representing the scattered and ejected electrons respectively. Here z_f and z_e are the effective charges seen by the scattered and ejected electrons respectively. Following Rudge and Schwartz (1966) we have taken $z_f = Z - 1$ and $z_e = Z$. In equation (6), $\chi_{k_a}(z_a, r)$ is decomposed into partial waves as

$$\chi_{k_{a}}(z_{a}, r) = 4\pi \sum_{\lambda=0}^{\infty} \sum_{\mu=-\lambda}^{\lambda} i^{\lambda} \frac{G_{\lambda}(k_{a}, z_{a}, r)}{k_{a} r} Y_{\lambda\mu}(\hat{r}) Y_{\lambda\mu}^{*}(\hat{k}_{a})$$
$$\times \exp\{-i\eta_{\lambda}(k_{a})\}, \qquad (7)$$

where $G_{\lambda}(k_{\alpha}, z_{\alpha}, r)$ is the λ th order regular Coulomb function (Abramowitz and Stegun 1972), $n_{\lambda}(k_{\alpha})$ is the λ th order Coulomb phase shift, and $Y_{\lambda\mu}(\hat{k}_{\alpha})$ is a spherical harmonic.

Following McDowell *et al.* (1973, 1974, 1975) in the DWPO method, the total scattering function $\psi_i^{\pm}(r_1, r_2)$ can be written as

$$\psi_{i}^{\pm}(r_{1}, r_{2}) = (1 \pm P_{12}) \{ \Phi_{1s}(r_{2}) + \Phi_{pol}(r_{1}, r_{2}) \} F^{\pm}(r_{1}), \qquad (8)$$

so that $\psi_i^{\pm}(r_1, r_2)$ is represented by a fully antisymmetrised polarised orbital function (Temkin and Lamkin 1961). Here P_{12} is the permutation operator which interchanges

$$\Phi_{1s}(\mathbf{r}) = R_{1s}(\mathbf{r}) Y_{00}(\hat{\mathbf{r}}), \qquad (9)$$

with

$$R_{1s}(r) = 2z^{\frac{3}{2}} \exp(-Zr).$$
 (10)

The distorted part of the target wavefunction can be written as (Temkin 1959)

$$\Phi_{\rm pol}(r_1, r_2) = -\pi^{-\frac{1}{2}} \frac{\epsilon(r_1, r_2)}{r_1} \frac{u_{1\rm s} \to p(r_2)}{r_2} \cos\theta_{12} \tag{11}$$

in the usual notation, with

$$u_{1s \to p}(r) = Z^{-\frac{1}{2}}(\frac{1}{2}Zr^{3} + r^{2})\exp(-Zr), \qquad (12)$$

$$\epsilon(r_{1}, r_{2}) = 1, \quad r_{1} > r_{2}$$

$$= 0, \quad r_{1} < r_{2}, \qquad (13)$$

and with θ_{12} the angle between r_1 and r_2 .

In the DWPO method the wavefunction $F^{\pm}(r_1)$ of the incident electron is determined by following the original polarised orbital procedure of Temkin and Lamkin (1961). Thus, making a partial wave expansion of $F^{\pm}(r_1)$, we get

$$F^{\pm}(r_{1}) = k_{i}^{-\frac{1}{2}} r_{1}^{-1} \sum_{l'=0}^{\infty} (2l'+1) i^{l'} \exp\left[i\{\delta_{l'} + n_{l'}(k_{i})\}\right]$$
$$\times u_{l'}^{\pm}(k_{i}, r) P_{l'}(\cos\theta_{1}), \qquad (14)$$

where for the initial 1s state $u_l^{\pm}(k_i, r)$ satisfies (McDowell *et al.* 1973)

$$\left(\frac{d^2}{dr^2} + k_i^2 - \frac{l'(l'+1)}{r^2} - 2V_{1s, 1s}(r) - 2V_{pol}(r)\right) u_l^{\pm}(k_i, r)$$

= $\pm X_r(r) r R_{1s}(r)$, (15)

with

$$V_{1s, 1s}(r) = -\frac{Z-1}{r} - \left(Z + \frac{1}{r}\right) \exp(-2Zr), \qquad (16)$$

$$V_{\text{pol}}(r) = -\frac{9}{4x^4} \{ 1 - (1 + 2x + 2x^2 + \frac{4}{3}x^3 + \frac{2}{3}x^4 + \frac{4}{27}x^5) \times \exp(-2x) \}, \qquad (17)$$

Here x = Zr and

$$X_{l'}^{\pm}(r) = (E_{1s} - k_i^2) \delta_{l',0} \int_0^\infty R_{1s}(t) u_{l'}^{\pm}(k_i, t) t \, \mathrm{d}t + \frac{2}{2l'+1} \int_0^\infty R_{1s}(t) u_{l'}^{\pm}(k_i, t) r_{l'}(t, r) t \, \mathrm{d}t, \qquad (18)$$

with

$$r_{l'}(r,r') = r_{<}^{l'}/r_{>}^{l'+1},$$
(19)

where $r_{<}$ and $r_{>}$ are the lesser and greater of r_{1} and r_{2} , E_{1s} is the ground state energy of He⁺, and $\delta_{l',0}$ is the Kronecker delta. We have solved equation (16) for $u_{l'}^{\pm}(k_{i}, r)$ subject to the boundary conditions

$$u_{l'}^{\pm}(k_{\rm i},0)=0, \qquad (20)$$

$$u_{\overline{r}}^{\pm}(k_{\rm i},r) \underset{r \to \infty}{\sim} k_{\rm i}^{-\frac{1}{2}} \sin\{\phi(r) + \delta_{\overline{r}}^{\pm}\}, \qquad (21)$$

$$\phi(r) \underset{r \to \infty}{\sim} k_{i} r - \frac{1}{2} l' \pi + \frac{Z - 1}{k_{i}} \ln 2 k_{i} r + n_{l'}, \qquad (22)$$

where $\delta_{l'}$ is the l'th order partial wave phase shift and $n_{l'}$ is the Coulomb phase shift:

$$n_{l'}(k_{\rm i}) = \arg \Gamma \left(l' + 1 - \frac{{\rm i}(Z-1)}{k_{\rm i}} \right).$$
 (23)

The scattering amplitude in the framework of the DWPO approximation can be written as

$$f_{ion}^{\pm}(k_{\rm f}, k_{\rm e}) = (2\pi)^{-\frac{5}{2}} \int \chi_{k_{\rm e}}^{*}(z_{\rm e}, r_{2}) \chi_{k_{\rm f}}^{*}(z_{\rm f}, r_{1}) \\ \times \left(-\frac{1}{r_{\rm 1}} + \frac{1}{r_{\rm 12}}\right) \psi_{\rm i}^{\pm}(r_{\rm 1}, r_{\rm 2}) \,\mathrm{d}r_{\rm 1} \,\mathrm{d}r_{\rm 2} \,.$$
(24)

Following McDowell et al. (1974, 1975) and Mazumdar (1983) the ionisation amplitude can be written as

$$f_{\rm ion}^{\pm}(k_{\rm f}, k_{\rm e}) = f_{\rm d}^{\pm}(k_{\rm f}, k_{\rm e}) \pm f_{\rm e}^{\pm}(k_{\rm f}, k_{\rm e}) + f_{\rm pd}(k_{\rm f}, k_{\rm e}), \qquad (25)$$

where $f_d^{\pm}(k_f, k_e)$, $f_e^{\pm}(k_f, k_e)$ and $f_{pd}^{\pm}(k_f, k_e)$ are respectively the direct, exchange and polarised direct (arising from the distorted part Φ_{pol} of the target wavefunction) amplitudes for ionisation:

$$f_{d}^{\pm}(\boldsymbol{k}_{f}, \boldsymbol{k}_{e}) = (2\pi)^{-\frac{5}{2}} \int \chi_{\boldsymbol{k}_{e}}^{*}(\boldsymbol{z}_{e}, \boldsymbol{r}_{2}) \chi_{\boldsymbol{k}_{f}}^{*}(\boldsymbol{z}_{f}, \boldsymbol{r}_{1}) \left(-\frac{1}{r_{1}} + \frac{1}{r_{12}}\right) \\ \times \boldsymbol{\Phi}_{1s}(\boldsymbol{r}_{2}) F^{\pm}(\boldsymbol{r}_{1}) d\boldsymbol{r}_{1} d\boldsymbol{r}_{2}, \qquad (26)$$

$$f_{pd}^{\pm}(\boldsymbol{k}_{f}, \boldsymbol{k}_{e}) = (2\pi)^{-\frac{5}{2}} \int \chi_{\boldsymbol{k}_{e}}^{*}(\boldsymbol{z}_{e}, \boldsymbol{r}_{2}) \chi_{\boldsymbol{k}_{f}}^{*}(\boldsymbol{z}_{f}, \boldsymbol{r}_{1}) \left(-\frac{1}{r_{1}} + \frac{1}{r_{12}}\right) \\ \times \boldsymbol{\Phi}_{pol}(\boldsymbol{r}_{1}, \boldsymbol{r}_{2}) F^{\pm}(\boldsymbol{r}_{1}) d\boldsymbol{r}_{1} d\boldsymbol{r}_{2}. \qquad (27)$$

We have carried out the partial wave analysis of $f_d^{\pm}(k_f, k_e)$ and $f_{pd}^{\pm}(k_f, k_e)$, and we can write (Mazumdar 1983)

$$f_{d}^{\pm}(k_{f}, k_{e}) = (4\pi)^{\frac{5}{2}} k_{i}^{-\frac{1}{2}} \sum_{lm} \sum_{\lambda} \sum_{r} i^{r-l-\lambda} (2l'+1) \\ \times \left(\frac{2l+1}{2\lambda+1}\right)^{\frac{1}{2}} Y_{lm}(\hat{k}_{e}) Y_{\lambda,-m}(\hat{k}_{f}) \exp\left[i\{\delta_{l'} + n_{l'}(k_{i}) + n_{l}(k_{e})\}\right] \frac{1}{2l+1} \binom{l}{-m} \frac{1}{2} \sum_{l} \frac{1}{2} \left(\frac{l}{-m} \frac{l'}{2} - \frac{\lambda}{2}\right) \binom{l}{2} \frac{l'}{2} \left(\frac{l}{2} - \frac{l'}{2} - \frac{\lambda}{2}\right) \\ \times \int_{0}^{\infty} u_{l'}^{\pm}(k_{i}, r_{i}) \frac{G_{\lambda}(k_{f}, z_{f}, r_{i})}{k_{f} r_{i}} \left(\int_{0}^{\infty} \frac{G_{l}(k_{e}, z_{e}, r_{2})}{k_{e}} + R_{1s}(r_{2}) r_{l}(r_{1}, r_{2}) r_{2} dr_{2} dr_{2} dr_{1}, \qquad (28)$$

$$f_{pd}^{\pm}(\boldsymbol{k}_{f}, \boldsymbol{k}_{e}) = -(4\pi)^{\frac{5}{2}} k_{i}^{-\frac{1}{2}} \sum_{lm} \sum_{\lambda} \sum_{l'} i^{l'-l-\lambda} (2l'+1) \\ \times \left(\frac{2l+1}{2\lambda+1}\right)^{\frac{1}{2}} Y_{lm}(\hat{\boldsymbol{k}}_{e}) Y_{\lambda,-m}(\hat{\boldsymbol{k}}_{f}) \exp\left[i\{\delta_{l'}+n_{l'}(\boldsymbol{k}_{i})+n_{\lambda}(\boldsymbol{k}_{f}) + n_{l}(\boldsymbol{k}_{e})\}\right] \\ + n_{l}(\boldsymbol{k}_{e})\} \frac{1}{2l+1} \binom{l}{-m} \frac{1}{0} \binom{l}{-m} \binom{l}{0} \frac{l'}{0} \binom{l}{0} \frac{l'}{0} \frac{u_{l'}^{\pm}(\boldsymbol{k}_{i}, \boldsymbol{r}_{1})}{r_{1}} \\ \times \frac{G_{\lambda}(\boldsymbol{k}_{f}, \boldsymbol{z}_{f}, \boldsymbol{r}_{1})}{\boldsymbol{k}_{f} r_{1}} \left[\int_{0}^{r_{1}} \frac{G_{l}(\boldsymbol{k}_{e}, \boldsymbol{z}_{e}, \boldsymbol{r}_{2})}{\boldsymbol{k}_{e} r_{2}} u_{1s \rightarrow p}(r_{2}) \left\{ \frac{2(l+1)}{2l+3} \left(\frac{r_{2}}{r_{1}}\right)^{l+2} + \frac{2l}{2l-1} \left(\frac{r_{2}}{r_{1}}\right)^{l} - \frac{2}{r_{1}} \delta_{l,1} r_{2}^{l} \right] dr_{1} \right] dr_{1} .$$
(29)

The quantities in the large parentheses are the usual Clebsch-Gordan coefficients (Rose 1963). According to Rudge and Schwartz (1966) the exchange amplitude is

given by

$$f_{e}^{\pm}(k_{f}, k_{e}) = f_{d}^{\pm}(k_{e}, k_{f}).$$
(30)

3. Numerical Methods

The integrodifferential equation satisfied by $u_{l'}^{\pm}(k_i, r)$ has been solved by using the Numerov method (Sloan 1964) with a step size of 0.02 up to r = 40 a.u., and higher values when required have been obtained by using the asymptotic form. The Coulomb functions have been obtained by solving the corresponding differential equations with a step size of 0.02 a.u. The program was run for smaller step sizes. Radial integrations occurring in $f_{ion}^{\pm}(k_f, k_e)$ have been performed up to r = 80 a.u. Special care was taken to ensure convergence with respect to angular momentum quantum numbers l, l' and λ . The maximum value of l was taken to be 6, whereas the maximum value of l' was varied from l' = 8 for E = 61.2 eV to l' = 12 for

Table 1. Total cross section Q_{ion} (in units of $\pi a_0^2/16$) for the e^--He^+ (1s) ionisation in different approximations

| | CBOX | CBX | DWPO |
|-------------|-------|-------|-------|
| Energy (eV) | | | |
| 61.2 | 0.215 | 0.213 | 0.196 |
| 68.0 | 0.392 | 0.366 | 0.347 |
| 82.4 | 0.666 | 0.580 | 0.547 |
| 122.4 | 1.002 | 0.834 | 0.784 |
| 163.2 | 1.072 | 0.896 | 0.864 |
| 217.6 | 1.035 | 0.881 | 0.842 |
| 272.0 | 0.962 | 0.832 | 0.802 |



Energy (eV)

Fig. 1. Total cross section Q_{ion} in units of 10^{-18} cm² for e^- -He⁺(1s) ionisation: solid curve, present DWPO results; dashed curve, CBX results of Rudge and Schwartz (1966); and dot-dash curve, CBOX results of Rudge and Schwartz (1966). The experimental results are from Peart *et al.* (1969).

E = 272.0 eV. For higher values of l' we replaced the higher order partial wave contributions by the CBX values of Rudge and Schwartz (1966). As a further check of our program we reproduced the CBX results of Rudge and Schwartz (1966).

4. Results and Discussion

The total cross section (TCS) for $e^--He^+(1s)$ ionisation in different approximations is tabulated in Table 1. In Fig. 1 we have plotted the present DWPO results together with the CBOX and CBX results of Rudge and Schwartz (1966) and the experimental results of Peart *et al.* (1969). We find that the present DWPO results are in good agreement with experiment. The sensitivity of the incident wave in predicting the TCS for $e^--He^+(1s)$ ionisation can be judged by comparing the present results with the CBX results. We find that the distortion of the incident wave brings the theoretical results closer to those of experiment.

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