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On the single- and double-ionization of He by protons and anti-protons

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Abstract. In this paper we present the calculations of: (a) the single-ionization cross section of He by protons and anti-protons in the incident energy range of about 10 keV–50 MeV, (b) the double-ionization cross sections by both projectiles in the energy rage of about 50 keV–20 MeV and (c) the ratio of double- to single-ionization in the energy range of 50 keV–20 MeV. The calculations have been performed in the two-coupled channel plane wave Born approximation, which is essentially the Born approximation that includes the final channel interaction between two electrons, in addition to the usual projectile–electron potential. The projectile has been represented by plane waves, and a correlated Hylleraas type of wavefunction has been used for the initial ground state. For the single-ionization case the final state electronic wavefunction is taken to be an anti-symmetrized product of a hydrogen-like (ls) and a continuum Coulomb wavefunction. For the double-ionization case, the final state wavefunctions of the two ejected electrons are taken to be Coulomb functions for calculating the matrix elements of the electron–projectile interaction, whereas plane waves are used for calculating the matrix elements of the electron–electron interaction. The calculated results are in reasonable agreement with the data in all three cases. The single-ionization cross section has also been calculated in the Lewis–Merzbacher approximation to determine the range of incident energy where it might represent a suitable approximation.

1. Introduction

In a series of experiments, Andersen *et al* (1986, 1987) have found that the ratio, R, of the double- to single-ionization of He by protons and anti-protons differ significantly in the incident energy range of a few tens of keV to a few tens of MeV. Subsequently, measured single- as well as double-ionization cross sections of He by protons (Puckett and Martin 1970, Shah and Gilbody 1985, 1982a, b, Shah *et al* 1989) and anti-protons are found to differ significantly from each other (Andersen *et al* 1989, 1990, Hvelplund *et al* 1994).

Prior to the series of experiments by Shah and Gilbody on the proton-induced single-ionization of He using crossed-beam coincidence technique, there have been many measurements of proton-induced single-ionization cross sections of He using the condenser-plate technique which are referred to by Shah and Gilbody (1985). In particular, Rudd *et al* (1983) have measured the single-ionization cross section of He by incident protons in the energy range of a few keV to 4000 keV. Their measurements are in general agreement with those of Shah and Gilbody (1985) for energies above 200 keV. The measurements of Puckett and Martin (1970) also agree with those of Shah and Gilbody (1985). It is, therefore, well established that the single-ionization cross section of He is different for incident protons and anti-protons.

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Similarly, the measurements of Shah and Gilbody (1985) of the double-ionization cross section of He by protons are in accord with the previous results of Puckett and Martin (1970) and hence it is established that the double-ionization cross section of He by incident protons and anti-protons are different.

These findings are significant because, within the framework of the Lewis–Merzbacher (LM) theory of plane wave Born approximation which denotes the projectile wavefunction in the incident and the outgoing channels by plane waves and considers only the electron–projectile interaction as perturbation, the single- and the double-ionization cross section in both cases should be the same. Consequently, the ratio, R, in the two cases should be the same.

In the Coulomb–Born approximation, used by Trefftz (1963) to study the single-ionization of OV and OV1 by electron impact, the wavefunction of the projectile in the final channel is represented by the Coulomb function. In that case, one expects, in principle, a difference in the ionization cross section induced by protons and anti-protons because of the difference in the signature of the charge in the Coulomb function for protons and anti-protons in the final channel. Similarly, in the distorted wave approximation, used by Malik and Trefftz (1961) to study the single-ionization of OV by electron impact, the single-ionization cross section of He by protons and anti-protons should, in principle, differ. In fact, the study of Fainstein *et al* (1987), which includes the distortion of the ejected electron due to the incident projectile in the eikonal approximation and a Coulomb wavefunction to describe the ejected electron as well as the projectile in the final channel (CDW-EIS: continuum-distorted-wave-eikonal-initial-state model), finds different single-ionization cross sections for incident protons and anti-protons. This difference is due to the signature of the charge of the projectile in the final channel in the two cases. Their calculations for incident anti-protons reasonably account for the data from about 15 keV to 3 MeV (Hvelplund *et al* 1994). Their calculations for incident protons reproduces the general trend of the observed cross section as a function of incident proton energy (Shah *et al* 1985, 1989) but differs by as much as 25% quantitatively (Andersen *et al* 1990). Unfortunately, no calculation of double-ionization cross sections of He in this approximation has been reported.

The theoretical calculation based on the classical-trajectory Monte Carlo (CTMC) method (Olson 1987, Schultz 1989) does not provide satisfactory agreement with the data (Hvelplund *et al* 1990) for the photon-induced single-ionization cross section of He. Calculations of the single-ionization cross section, based on an improved version of this model (Montemayor and Schiwietz 1989, Meng *et al* 1993) that includes correlation between the two electrons of He in terms of screening potentials (the model is termed dCTMC), yield cross sections of 0.404 and 0.293 $\mathring{A}^2$ for 300 and 500 keV incident protons, respectively, and 0.327 and 0.251 $\mathring{A}^2$ for incident anti-photons of 300 and 500 keV, respectively. The observed data for the incident proton energies of 260, 320 and 500 keV amu^{-1} are, respectively, 0.587 ± 0.011, 0.516 ± 0.09 and 0.370 ± 0.015 $\mathring{A}^2$ (Shah and Gilbody 1985) and for the incident anti-proton energies of 270.1, 326.3 and 503. keV are, respectively, 0.471 ± 0.08, $0.437\,0.08$ and 0.354 ± 0.08 $\mathring{A}^2$ (Hvelplund *et al* 1994). Their double-ionization cross sections calculated only for the 500 keV incident protons and anti-protons overestimate significantly the proton-induced double-ionization data at these energies and slightly underestimate the corresponding anti-proton data.

Ford and Reading (1988, 1990, 1994) and Reading and Ford (1987a, b) have approached the problem from the time-dependent viewpoint. Their model, termed the forced-impulse method (FIM), breaks up the time development into small segments. Within a given segment, the electrons are treated in an uncorrelated fashion but between the segments the correlation is considered. Their earlier calculations, done for incident energies higher than a few hundred keV, including the s and p electron orbitals in the He wavefunction, are in qualitative agreement with the proton data but falls short on the ratio of double- to single-ionization by anti-protons. However, their latest calculation done only at 300, 500 and 1000 keV incident energies (Ford and Reading 1994) estimating the contributions of the 9d orbitals to the single- and double-ionization are in reasonable quantitative agreement with the data around these energies. For example, their estimated cross sections for the single-ionization by incident proton are 0.498, 0.346 and 0.203 $\mathring{A}^2$ at energies of 300, 500 and 1000 keV, respectively, which are close to the observed values of 0.516 ± 0.009, 0.370 ± 0.015 and 0.226 ± 0.008 $\mathring{A}^2$ (Shah and Gilbody 1985) measured at incident energies of 320, 500 and 1000 keV amu^{-1}, respectively. Similarly, they estimate the single-ionization cross sections by incident anti-proton of energies 300, 500 and 1000 keV to be 0.458, 0.331 and 0.188 $\mathring{A}^2$, respectively. These are close to the observed values (Hvelplund *et al* 1994, Andersen *et al* 1990) of 0.471 ± 0.02, 0.437 ± 0.02, 0.354 ± 0.02 and $0.195 \pm 0.01\mathring{A}^2$ at incident energies of 270.1, 326.3, 503.6 and 1130 keV, respectively. So far, calculations at other energies, particularly the lower ones, have not been reported, although the measurements are available.

Ford and Reading (1994) have calculated the double-ionization cross sections by incident protons and anti-protons only at three energies, namely at 300, 1000 and 6000 keV and estimated them at 500, 3000 and 10 000 keV. Their calculated results for the 300, 500 and 1000 keV incident-proton energies are in good agreement with the data of Shah and Gilbody (1985) taken at 326, 500 and 1000 keV amu^{-1}. However, their calculated cross sections for the 300 and 500 keV incident anti-protons differ about 10–20% from the data taken at 270, 326 and 503 keV incident energies (Andersen *et al* 1986, 1987, Hvelplund *et al* 1994). No calculation has been reported for lower incident energies in the FIM. For a proper understanding of the underlying reaction mechanism associated with the ionization process, it is important to understand the low-energy data at least in the 100–300 keV region.

The early calculations of single-ionization by Bell and Kingston (1969) using plane wave Born approximation that approximates the electron–projectile interaction as dipole or the corresponding velocity operator (so called Bethe (1930) approximation) and uses a correlated ground-state wavefunction, do not agree with the data. In particular, the maximum of the cross section is not accounted for (Shah and Gilbody 1985). Of course, the anti-proton-induced single-ionization cross section is equal to that by protons in this approximation, and the observed difference in the data in two cases cannot be explained.

Toburen *et al* (1978) have calculated the single-ionization cross section at 300, 500 and 1000 keV incident-proton energies in the LM approximation, except replacing the initial hydrogenic He ground-state wavefunction by Herman and Skillman's (1963) parametrized Hartree–Fock wavefunction and the Sommerfeld Coulomb wavefunction for the ejected electron by a distorted wave (Manson *et al* 1975). Their calculated result agrees with the data of Rudd *et al* (1983) at 300 keV but is slightly higher than the data at 500 and 1000 keV, and differs significantly from the 100 keV data. Earlier, Lewis and Merzbacher (1958) presented the single-ionization cross section in the LM approximation from the threshold to 200 keV, with limited agreement to the data.

Das (1994) and Das and Malik (1996) have analysed the single- and double-ionization of He by protons and anti-protons using the coupled-channel approach (Mott and Massey 1965, Malik and Trefftz 1961) in the lowest order, i.e. restricting it only to two channels and representing the projectile wavefunction in both channels by plane waves. These calculations, reported only for a few very low and high energies, are in good agreement with the data of the single- and double-ionization by both types of projectiles. In this paper, we extend the calculations of: (a) the single-ionization of He by protons and anti-protons from

10 keV to 50 MeV incident energies, (b) the double-ionization of He by each projectile from a few tens of keV to 20 MeV incident energies and (c) the ratios of the two. We also present the single-ionization cross section in the LM approximation in the 10 keV–50 MeV range. In section 3, we compare them with the available data.

2. Theory

The Schroedinger equation for an incident projectile and a He atom in the centre-of-mass system of the incident particle and the nucleus of He may be written as

$$\left[-\frac{\hbar^2}{2\mu}\nabla_R^2 - \frac{\hbar^2}{2m}(\nabla_1^2+\nabla_2^2) - \left(\frac{\mp Ze^2}{R}\right) - \frac{Ze^2}{r_1} - \frac{Ze^2}{r_2} + \frac{e^2}{r_{12}} \mp \frac{e^2}{|\boldsymbol{R}-\boldsymbol{r}_1|} \mp \frac{e^2}{|\boldsymbol{R}-\boldsymbol{r}_2|} - E\right]\Psi(\boldsymbol{R},\boldsymbol{r}_1,\boldsymbol{r}_2) = 0. \tag{1}$$

In (1) μ and m are the reduced masses of the projectile and the electrons, respectively, with respect to the He nucleus, respectively. $\boldsymbol{r}_1$, $\boldsymbol{r}_2$ and $\boldsymbol{R}$ are the coordinates of the electrons 1 and 2 and the projectile with respect to the centre of mass, respectively. The minus and the plus signs refer, respectively, to the incident proton and the anti-proton. In (1) $r_{12} = |\boldsymbol{r}_1 - \boldsymbol{r}_2|$, is the interelectronic distance.

One may expand $\Psi(\boldsymbol{R},\boldsymbol{r}_1,\boldsymbol{r}_2)$ in the following orthonormal set

$$\Psi(\boldsymbol{R},\boldsymbol{r}_1,\boldsymbol{r}_2) = \sum_n F_n(\boldsymbol{R})\sum_m \Psi_{mn}(\boldsymbol{r}_1,\boldsymbol{r}_2). \tag{2}$$

In view of the fact that the two electrons are far apart in the final channel and do not interact, we define the orthonormal set to be the eigenfunctions of the following Hermitian Hamiltonian:

$$H_0\Psi_{mn} \equiv \left[-\frac{\hbar^2}{2m}(\nabla_1^2+\nabla_2^2) - \frac{Ze^2}{r_1} - \frac{Ze^2}{r^2}\right]\Psi_{nm}(\boldsymbol{r}_1,\boldsymbol{r}_2) = E_m\Psi_{mn}(\boldsymbol{r}_1,\boldsymbol{r}_2). \tag{3}$$

The above Hamiltonian accurately represents the asymptotic situation in the final channel where the ejected electron is far away from the He^+ ion for the single-ionization case and both the ejected electrons are away from each other in the double-ionization case. Hence, the $e^2/\boldsymbol{r}_{12}$ term is negligible.

One may obtain the following equation for $F_n(\boldsymbol{R})$ by taking the scalar product of (1) with respect to Ψ_{mn} and integrating over the coordinates $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$:

$$\begin{aligned}\left\{\frac{\hbar^2}{2m}\nabla^2 + (E-E_n) \mp \frac{Ze^2}{R}F_n(\boldsymbol{R})\right\}F_n(\boldsymbol{R}) &= \int \mathrm{d}\boldsymbol{r}_1\,\mathrm{d}\boldsymbol{r}_2 \sum_m \Psi^*_{mn}(r_1,r_2)\left\{\mp\frac{Ze^2}{|\boldsymbol{R}-\boldsymbol{r}_1|} \mp \frac{Ze^2}{|\boldsymbol{R}-\boldsymbol{r}_2|} + \frac{e^2}{r_{12}}\right\}\\ &\quad\times \sum_{n'\neq n} F_n(\boldsymbol{R})\sum_{m'}\Psi_{m'n'}(r_1,r_2).\end{aligned} \tag{4}$$

The orthogonality condition on Ψ_{nm} has been used in deriving (4). Using

$$k_n^2 = \frac{2m}{\hbar^2}(E-E_n) \tag{5}$$

one gets

$$\left(\nabla^2 + k_n^2 \mp \frac{Ze^2}{R}\right) F_n(\boldsymbol{R}) = \frac{2m}{\hbar^2} \int \mathrm{d}\boldsymbol{r}_1\, \mathrm{d}\boldsymbol{r}_2 \sum_m \Psi^*_{mn}(\boldsymbol{r}_1, \boldsymbol{r}_2) \times \left\{\mp \frac{Ze^2}{|\boldsymbol{R} - \boldsymbol{r}_2|} \mp \frac{Ze^2}{|\boldsymbol{R} - \boldsymbol{r}_2|} + \frac{e^2}{r_{12}}\right\} \sum_{n' \neq n} F_{n'}(\boldsymbol{R}) \sum_{m'} \Psi_{m'n'}(\boldsymbol{r}_1, \boldsymbol{r}_2). \tag{6}$$

Equation (6) represents an infinite set of coupled equations, and suitable approximations are needed before the actual calculations could be carried out.

The above equation is to be solved with the following boundary condition in the final channel as $\boldsymbol{R}$ goes to infinity:

$$F_n(\boldsymbol{R}) \rightarrow f_n(\theta, \vartheta) \frac{\mathrm{e}^{\mathrm{i}(k_n R - \eta \ell n 2 k_n R)}}{R} \tag{7}$$

with $\eta = \mu Z e^2/\hbar k_n$, Z being the projectile charge. $f_n(\theta, \vartheta)$ is the scattering amplitude in the channel n at an angle (θ, ϑ) defined with respect to the direction of incident momentum. Following Mott and Massey (1965), one may obtain the following expression for the differential cross section:

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = |f_n(\theta, \vartheta)|^2 = \frac{4\pi^2\mu^2}{h^4} \frac{k_n}{k_0} \int\int\int \mathrm{d}\boldsymbol{r}_1\, \mathrm{d}\boldsymbol{r}_2\, \mathrm{d}\boldsymbol{R} F^*_{nh}(\boldsymbol{R}) \times \sum_m \Psi^*_{nm}(\boldsymbol{r}_1, \boldsymbol{r}_2) H_{\mathrm{int}}(\boldsymbol{R}, \boldsymbol{r}_1, \boldsymbol{r}_2) \sum_{n'm'} F_{n'}(\boldsymbol{R}) \Psi_{m'}(\boldsymbol{r}_1, \boldsymbol{r}_2)|^2 \tag{8}$$

with

$$H_{\mathrm{int}}(\boldsymbol{R}, \boldsymbol{r}_1, \boldsymbol{r}_2) = \mp \frac{Ze^2}{|\boldsymbol{r}_1 - \boldsymbol{R}|} \mp \frac{Ze^2}{|\boldsymbol{r}_2 - \boldsymbol{R}|} + \frac{e^2}{r_{12}} \tag{9}$$

k_0 in (8) is the incident channel wavenumber and $F^*_{nh}(\boldsymbol{R})$ is the solution of the homogeneous part of (6) compatible with the asymptotic boundary condition (7), i.e. the outgoing Coulomb wavefunction for protons or anti-protons.

The total single-ionization cross section, σ^+, is obtained by integrating over the solid angle $\mathrm{d}\Omega$.

It is important to note that the expression (8) is exact and the e^2/r_{12} term is to be included in calculating the matrix elements. In case the electron–projectile interaction is switched off, the projectile wavefunction is zero and hence, matrix elements of e^2/r_{12} and the cross section are zero, i.e. there is no transition, as it should be.

Since the energy interval considered in this work is significantly larger than the thresholds for the single- and double-ionization, we consider explicitly only two channels in our calculation, namely the initial and the final ones. In this two-channel approximation, the summation over n in (2) has two terms and the initial and final channels are denoted as $F_0(\boldsymbol{R})$ and $F_n\boldsymbol{R}$, respectively. The summation over n' in (8) reduces to the following term:

$$\sum_{n'm'} F_{n'}(\boldsymbol{R}) \Psi_{n'm'}(\boldsymbol{R}, \boldsymbol{r}_1, \boldsymbol{r}_2) \cong F_0(\boldsymbol{R}) \sum_{m'} \Psi_{0m'}(\boldsymbol{r}_1, \boldsymbol{r}_2) = F_0(\boldsymbol{R}) \Psi_g(\boldsymbol{r}_1, \boldsymbol{r}_2) \tag{10}$$

Ψ_g in (10) is the correlated ground-state wavefunction of He.

In this approximation the differential cross section is given by

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \frac{4\pi^2\mu^2}{h^4} \frac{k_n}{k_0} \left| \int \mathrm{d}\boldsymbol{r}_1\, \mathrm{d}\boldsymbol{r}_2\, \mathrm{d}\boldsymbol{R} F^*_{nh}(\boldsymbol{R}) \Psi_n(\boldsymbol{r}_1, \boldsymbol{r}_2) H_{\mathrm{int}}(\boldsymbol{R}, \boldsymbol{r}_1, \boldsymbol{r}_2) F_0(\boldsymbol{R}) \Psi_g(\boldsymbol{r}_1, \boldsymbol{r}_2) \right|^2. \tag{11}$$

In case $F_{nh}(\boldsymbol{R})$ and $F_0(\boldsymbol{R})$ are taken, respectively, to be Coulomb and plane waves, this approximation is equivalent to the Coulomb–Born approximation used by Trefftz (1963) for the single-ionization of oxygen-ions by electron.

The two-channel plane wave Born approximation (2cPWBA) is obtained by replacing F_0 and F_{nh} by the plane wavefunction in respective channels. The differential cross section in the 2cPWBA is then given by

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \frac{4\pi^2\mu^2}{h^4}\frac{k_n}{k_0}\left|\int \mathrm{d}\boldsymbol{r}_1\,\mathrm{d}\boldsymbol{r}_2\,\mathrm{d}\boldsymbol{R}\exp[\mathrm{i}(k_0\hat{n}_0 - k_n\hat{n})\cdot\boldsymbol{R}]\right.$$
$$\left.\times\Psi_n^*(\boldsymbol{r}_1,\boldsymbol{r}_2)H_{\mathrm{int}}(\boldsymbol{R},\boldsymbol{r}_1,\boldsymbol{r}_2)\Psi_g(\boldsymbol{r}_1,\boldsymbol{r}_2)\right|^2. \qquad (12)$$

The total cross section is obtained by integrating over $\mathrm{d}\Omega$. In (12), $\hat{n}_0$ and $\hat{n}$ are unit vectors in the direction of momenta in the incident and the final channels, respectively.

For the single-ionization case, $\Psi_n(\boldsymbol{r}_1,\boldsymbol{r}_2)$ is a properly anti-symmetrized product of a bound (ls) and an outgoing hydrogen-like continuum wavefunction. For the double-ionization case, it is a product of properly anti-symmetrized two hydrogen-like continuum wavefunctions. $\Psi_g(\boldsymbol{r}_1,\boldsymbol{r}_2)$ is the ground-state singlet wavefunction of He. Since the interaction is spin independent, $\Psi_n(\boldsymbol{r}_1,\boldsymbol{r}_2)$ represents a singlet state.

The LM approximation is obtained by: (a) replacing Ψ_g with a product of two hydrogen-like (ls) wavefunctions and (b) neglecting the e^2/r_{12} term in $H_{\mathrm{int}}(\boldsymbol{R},\boldsymbol{r}_1,\boldsymbol{r}_2)$. This will be used for the single-ionization case.

The Bethe approximation, sometimes denoted as the zero-order or lowest-order Born approximation, is obtained by: (a) replacing Ψ_g in (12) with a product of two (ls) hydrogen-like wavefunctions, (b) omitting e^2/r_{12} from H_{int} and (c) keeping only terms up to dipole in the expansion of the electron–projectile interaction. This approximation has usually been applied for the single-ionization case.

Because the interaction term $H_{\mathrm{int}}(\boldsymbol{R},\boldsymbol{r}_1,\boldsymbol{r}_2)$ given by (9) is different for incident protons and anti-protons, the calculated single-ionization cross section in the 2cPWBA for the two cases should differ, in principle, from each other. On the other hand, in the LM and Bethe approximations, they are the same.

The initial-state wavefunction used to calculate both the single- and double-ionization is the following correlated wavefunction due to Hylleraas (1930):

$$\Psi_g(\boldsymbol{r}_1,\boldsymbol{r}_2) = N_{\exp}(-(\gamma/a_{\mathrm{o}})(r_1+r_2))(1+cr_{12}^2). \qquad (13)$$

In (13) N and a_{o} are, respectively, the normalization constant and the Bohr radius. γ and c, determined from the Raleigh–Ritz variational principle, are 1.69 and 0.142, respectively. The variational ground-state energy is -78.28 eV, which is very close to the observed value of -78.62 eV.

For the single-ionization case, the final-state electronic wavefunction, $\Psi_n(\boldsymbol{r}_1,\boldsymbol{r}_2)$ in the 2cPWBA is taken to be a product of a hydrogenic (ls) wavefunction with an effective charge of 2.0 and a continuum Coulomb wavefunction in the Sommerfeld representation (Wentzel 1929, Bethe 1930, Sommerfeld 1931, Massey and Mohr 1933) with an effective charge of 1.09.

Calculations of the single-ionization cross section in the LM approximation have been performed by taking the electronic wavefunction in the initial state to be a product of two hydrogenic (ls) functions, each having an effective charge of 1.6875 along with the same final-state electronic wavefunction used in the 2cPWBA.

For the double-ionization case, the electronic wavefunction in the final channel, $\Psi_n(\boldsymbol{r}_1,\boldsymbol{r}_2)$, is taken to be a product of two continuum Coulomb wavefunctions having two units of charge in the Sommerfeld representation for calculating matrix elements of the electron–projectile interaction and a product of two outgoing plane waves for calculating matrix elements of e^2/r_{12}. The latter approximation is motivated by the fact that, in the case of single-ionization, matrix elements of the e^2/r_{12} term, calculated with the plane and Coulomb wavefunctions for the ejected electron, yield about the same numerical value (Das and Malik 1996) in the entire energy range.

3. Results and Discussion

3.1. Single-ionization

3.1.1. The LM approximation. In table 1, we present our calculated results in the LM approximation for the incident energy range of 10 keV–50 MeV for both the incident protons and anti-protons. In the energy range of 10–200 keV, our calculations are in agreement with those of Lewis and Merzbacher (1958) which also serve as a check to our numerical code.

Table 1. Comparison of the calculated single-ionization cross section of He by proton in the LM approximation (column 2) and the 2cDWBA (column 3) with the selected data in experiments of Shah and Gilbody (1981, 1985), Shah *et al* (1989) and Puckett and Martin (1970).

Energy (keV)	σ (LM) (10^{-16} cm^2)	σ (this work) (10^{-16} cm^2)	σ (Shah) (10^{-16} cm^2)	σ (Puckett) (10^{-16} cm^2)
10.00	0.088	0.081		
11.09			0.067 ± 0.003	
19.15			0.192 ± 0.006	
20.00	0.312	0.299		
28.22			0.340 ± 0.014	
30.00	0.512	0.499		
50.00	0.752	0.739		
64.51			0.750 ± 0.023	
70.00	0.847	0.833		
100.00	0.859	0.850		
100.79			0.845 ± 0.046	
131.03			0.809 ± 0.012	
150.00				0.880
200.00	0.702	0.692		0.718
200.59			0.693 ± 0.017	
300.00	0.572	0.558		0.510
400.00				0.429
403.18			0.441 ± 0.009	
500.00	0.410	0.402		0.350
503.97			0.370 ± 0.015	
600.00				0.314
700.00	0.324	0.313		0.273
900.00				0.227
1 000.00	0.249	0.237		0.207
1 000.79			0.226 ± 0.008	
2 000.00	0.144	0.133		
2 000.79			0.130 ± 0.001	
2 398.90			0.112 ± 0.001	
5 000.00	0.061	0.059		
7 000.00	0.044	0.043		
9 000.00	0.040	0.034		
10 000.00	0.032	0.031		
30 000.00	0.016	0.011		
40 000.00	0.010	0.008		
50 000.00	0.007	0.006		

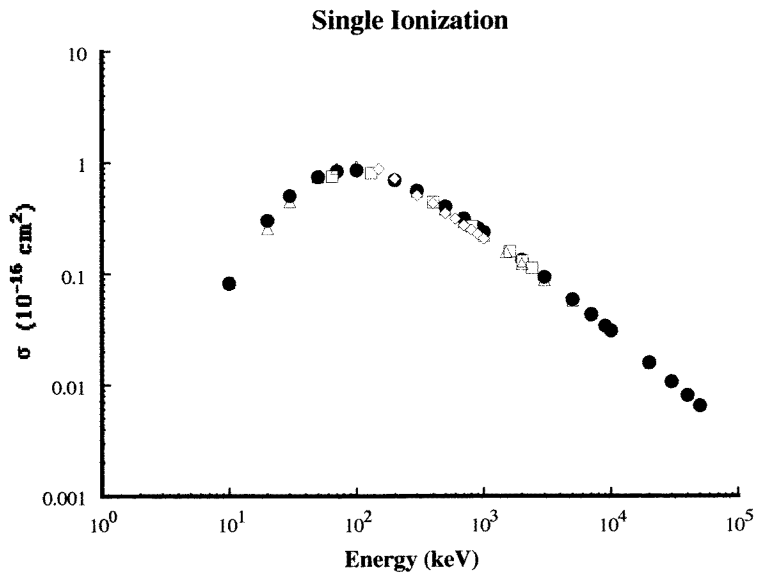

Figure 1. Comparison between the calculated single-ionization cross section of He by protons done in the LM approximation and selected data: ●, this work (p^+); □, Shah and Gilbody (1981, 1985) and Shah *et al* (1989); △, Rudd *et al* (1983); ◊, Puckett and Martin (1970).

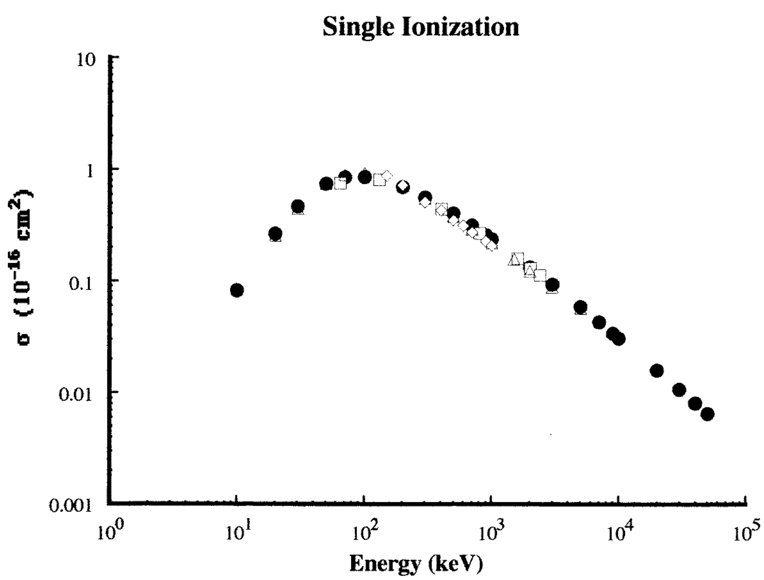

Figure 2. Comparison between the calculated single-ionization cross section of He by protons done in the 2cDWBA, denoted by ●, with selected data referred to in figure 1.

In figure 1 the data of Shah and Gilbody (1981, 1982a, b, 1985), Shah *et al* (1989) and Rudd *et al* (1983) for the single-ionization cross section of He by proton have been presented as a function of incident energies and compared with our calculation in the LM approximation. The theory can account for the data satisfactorily for incident energies greater than a few hundred keV. At lower energies there is room for improvement.

3.1.2. The 2cPWBA for the incident proton. In table 1, we have also presented our calculation for the single-ionization cross section of He by incident protons in the energy range of 10 keV–50 MeV in the two-channel plane wave Born approximation. In general, the calculated cross sections in the 2cPWBA are lower than those obtained in the LM approximation. The difference is about 10% below 50 keV and above 30 MeV and only a few per cent at other energies. In figure 2, we have compared our calculation with the data and the agreement is quite good in the entire energy range. In particular, the agreement between the theory and the experiment has improved significantly at lower energies compared to those calculated in the LM approximation.

Table 2. Comparison of the calculated single-ionization cross section of He by anti-proton in the 2cDWBA (column 2) with the selected data (column 3) of the Aarhus group (Andersen *et al* 1990, Hvelplund *et al* 1994).

Energy (keV)	σ (this work) (10^{-16} cm^2)	σ (Aarhus data) (10^{-16} cm^2)
10.00	0.106	
12.90		0.199 ± 0.037
20.00	0.323	
24.20		0.473 ± 0.038
30.00	0.526	
34.60		0.591 ± 0.027
50.00	0.767	
53.90		0.741 ± 0.030
70.00	0.861	
100.00	0.876	
101.60		0.645 ± 0.026
194.40		0.528 ± 0.020
200.00	0.718	
270.10		0.471 ± 0.019
300.00	0.582	
326.30		0.437 ± 0.017
500.00	0.425	
645.00		0.310 ± 0.022
700.00	0.336	
1 000.00	0.261	
1 130.00		0.195 ± 0.014
2 000.00	0.156	
2 470.00		0.105 ± 0.012
2 918.00		0.099 ± 0.012
3 000.00	0.116	
5 000.00	0.082	
7 000.00	0.066	
9 000.00	0.057	
10 000.00	0.053	
30 000.00	0.033	
40 000.00	0.031	
50 000.00	0.029	

3.1.3. The 2cPWBA for the incident anti-protons. In table 2, we have presented our calculation in the 2cPWBA for incident anti-protons in the energy range of 10 keV–50 MeV. They are compared with the observed single-ionization cross section in figure 3. The calculation reproduces the general energy dependence of the cross section and the data

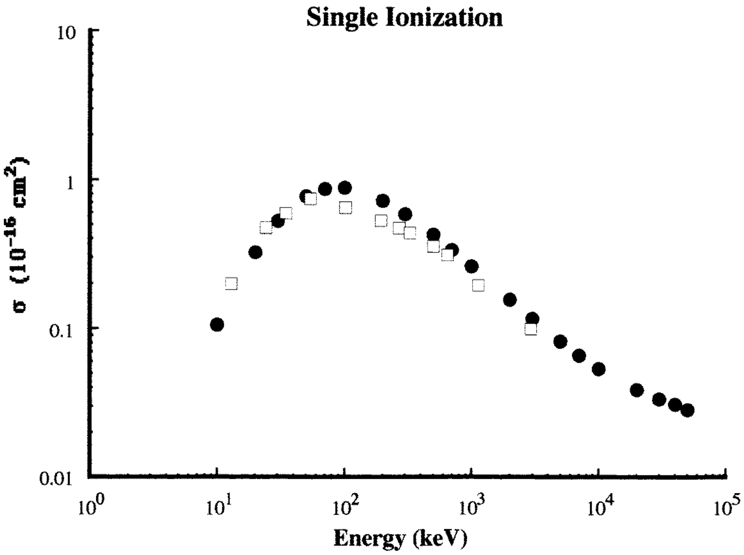

Figure 3. Comparison between the calculated single-ionization cross section of He by anti-protons done in the 2cDWBA and selected data of the group primarily based at Aarhus. □, Aarhus group data (Andersen *et al* 1990, Hvelplund *et al* 1994); ●, this work (p^-).

quite well. However, the calculated values between 80 and 300 keV are somewhat higher than the data. The calculated cross section for incident anti-protons is always higher than that for protons, but the difference is insignificant in the energy range of 70–2000 keV.

3.1.4. General discussion. For the proton-induced single-ionization of He, our calculation can reasonably account for the observed cross section in the entire energy range considered here. The agreement between the data and our calculation is slightly better than the one between the data and the calculation of Fainstein *et al* (1987) particularly below 150 keV and above 1000 keV. The Bethe approximation used by Bell and Kingston (1969) is inadequate at lower energies. The calculated values in the 2cPWBA agree with the data somewhat better than the calculations in the dCTMC (Meng *et al* 1993) and in the FIM approximations (Ford and Reading 1994). The LM approximation used by us is very similar to the method of Toburen *et al* (1978) and Manson *et al* (1975), except for the initial electronic wavefunction, and the numerical cross sections in the two cases are very close.

The contribution to the cross section from the matrix elements of the e^2/r_{12} term for the proton case is only significant at low energies, i.e. below 100 keV. In table 3, we have compared calculations in the 2cPWBA done using plane waves for the ejected electron instead of the Coulomb wavefunction to compute matrix elements of the e^2/r_{12} term, and they do not differ significantly. It is, therefore, sufficient to evaluate matrix elements of the e^2/r_{12} term using a plane wavefunction for the ejected electron, instead of the Sommerfeld representation of the Coulomb wavefunction. The use of a plane wavefunction for the ejected electron simplifies the calculation considerably.

For the incident anti-proton case, the observed data agree very well with our calculation for incident energies greater than about 200 keV. At lower energies, the calculations of Fainstein *et al* (1987) are in somewhat better agreement with the data compared with ours. The data are in better agreement with our calculation compared with those done in the FIM

Table 3. Comparison between the calculations of the single-ionization cross section of He by p^+ done in the 2cPWDA (column 3) and the approximation where the plane wavefunction is used for the ejected electron in evaluating the matrix element of e^2/r_{12} (column 2).

Energy (keV)	σ (plane wave) (10^{-16} cm^2)	σ (Sommerfeld[a]) (10^{-16} cm^2)
10.00	0.082	0.081
20.00	0.302	0.299
30.00	0.503	0.499
50.00	0.745	0.740
70.00	0.838	0.833
100.00	0.855	0.850
200.00	0.695	0.692
300.00	0.561	0.558
500.00	0.403	0.402
700.00	0.315	0.313
1 000.00	0.238	0.237
2 000.00	0.133	0.133
3 000.00	0.093	0.093
5 000.00	0.059	0.059
7 000.00	0.043	0.043
9 000.00	0.034	0.034
10 000.00	0.031	0.031
30 000.00	0.011	0.011
40 000.00	0.008	0.008
50 000.00	0.007	0.006

[a] Sommerfeld 1931.

(Ford and Reading 1994) and in the dCTMC (Meng *et al* 1993).

The 2cPWBA theory predicts that at very high incident energies, i.e. energies above a few MeV, the single-ionization cross section of He by anti-proton should be higher than that by incident proton so long as the non-relativistic description remains valid. This is the consequence of the difference in the perturbed potential, (9) in two cases. The data are available up to only about 2.5 MeV for the incident proton (Shah *et al* 1989) and 3.0 MeV for the incident anti-proton (Andersen *et al* 1990) and seem to bear out this theoretical projection. It would certainly be most interesting to have data at higher incident energies.

At incident energies lower than about 100 keV, our calculated cross section for incident anti-proton lies a little higher than those for protons, whereas the data indicate the situation to be the opposite. At this incident energy region, the difference in Coulomb distortion in the two cases is likely to play an important role. In addition, the possibility of resonances for the anti-proton–helium system may have to be considered. In the first approximation, the location of such resonances is determined by the eigenenergies of the homogeneous part of (4) (Malik 1992). Clearly, there should be no resonance for the incident-proton case since the (proton–He) system is unbound. On the other hand, the (anti-proton–He) system has bound states, the energies of which are very approximately given by $E = -(20.0\ \mathrm{keV})Z^2/n^2$ in the hydrogen-like approximation. Hence, the resonances could contribute to the cross section in the region of a few tens of keV for the anti-proton case and the spacing of these resonances should be from about one-tenth to a few keV. It is more interesting to note that the measured single-ionization cross section for the incident proton in the energy range of a few tens of keV is a smooth function of energy (Shah *et al* 1989) which is expected in the absence of resonances but the same for incident anti-proton seems to exhibit some structure (Hvelplund *et al* 1994) as expected in the presence of resonances. It would be

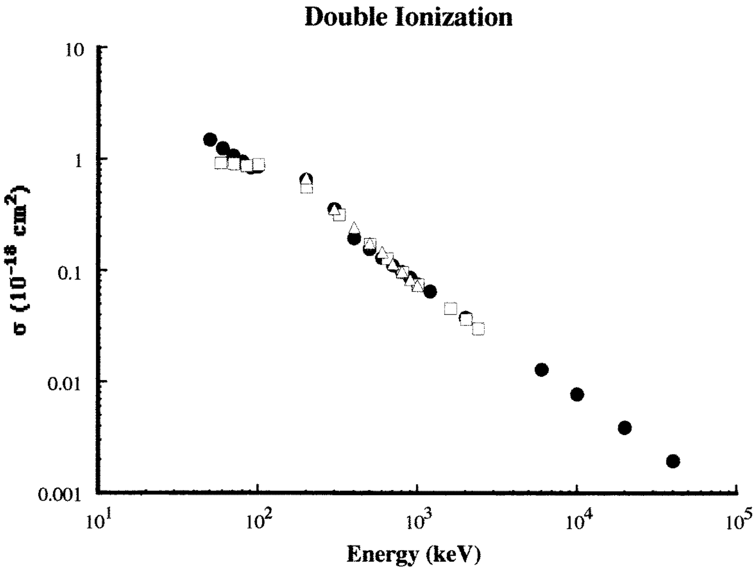

Figure 4. Calculated double-ionization cross section of He by protons, denoted by ●, is plotted as a function of proton incident energy and compared with the selected data: □, Shah and Gilbody (1982a, b, 1985) and Shah *et al* (1989); △, Puckett and Martin (1970).

most interesting to establish whether such structures are actually present for the anti-proton case and represent resonances.

3.2. Double-ionization and the ratio

3.2.1. Proton-induced double-ionization and the ratio. In table 4 and figure 4, we have presented our calculated results for the double-ionization cross section in the incident-proton energy range of about 50 keV–20 MeV and compared them with the measurements of Shah and Gilbody (1985), Shah *et al* (1989) and Puckett and Martin (1970). The measurements extend from about 16 to 2400 keV, although the data for energies below 50 keV have not been plotted. The calculation accounts for the energy dependence and the magnitude of the observed cross section from 80–2400 keV very well. Below 80 keV the calculated values for the cross section seem to be slightly higher than the data which, however, have large errors, typically 10%. The observed cross section seems to be rather flat from 40 to 100 keV, but not the calculated values. It would be most interesting to refine the measurement and extend the data to lower energies where the Coulomb distortion of the projectile in the final channel and multi-channel effects are expected to be important.

Meng *et al* (1993) have calculated double-ionization cross sections in the dCTMC method at two energies. Their calculated values are 7.3×10^{-19} cm^2 and 4.1×10^{-19} cm^2 for 300 and 500 keV incident energies, respectively, and are considerably larger than our calculated values and the observed data. Calculations and estimates of Ford and Reading (1988, 1994) for the 300, 500, 1000 and 3000 keV incident energies are about 10% lower than our results and slightly lower than the observed values, but their calculations for the 6.0 and 10.0 MeV agree with our results.

In table 6 and figure 6 we have presented our calculated and the observed ratios of double- to single-ionization cross sections for the incident protons in the energy range of

Table 4. Comparison between the calculated double-ionization cross section of He by proton, σ (this work), and the selected data, σ (Shah) and σ (Puckett).

Energy (keV)	σ (this work) (10^{-18} cm^2)	σ (Shah[a]) (10^{-18} cm^2)	σ (Puckett[b]) (10^{-18} cm^2)
50.00	1.496		
58.46		0.920 ± 0.240	
60.00	1.253		
70.00	1.079		
70.56		0.910 ± 0.190	
80.00	0.947		
80.67		1.057 ± 0.101	
84.67		0.870 ± 0.180	
90.00	0.844		
100.00	0.863		
100.79		$0.890 \pm 0.180^*$	
150.00			0.970
200.00	0.659		0.678
201.59		0.560 ± 0.017	
300.00	0.357		0.356
322.54		0.315 ± 0.022	
400.00	0.193		0.242
402.18		0.236 ± 0.012	
500.00	0.155		0.176
503.97		0.172 ± 0.008	
600.00	0.129		0.146
645.08		0.127 ± 0.001	
700.00	0.111		0.114
800.00	0.097		0.098
806.35		0.096 ± 0.005	
900.00	0.086		0.083
1 000.00	0.076		0.073
1 007.90		0.075 ± 0.003	
1 612.70		0.045 ± 0.004	
2 000.00	0.038		
2 015.90		0.037 ± 0.004	
2 398.90		0.030 ± 0.002	
3 000.00	0.024		
4 000.00	0.019		
5 000.00	0.016		
6 000.00	0.013		
7 000.00	0.011		
8 000.00	0.010		
9 000.00	0.009		
10 000.00	0.008		
30 000.00	0.003		
40 000.00	0.002		
50 000.00	0.002		

[a] Shah and Gilbody (1982a, b, 1985).
[b] Puckett and Martin (1970).

50 keV–20 MeV. The calculation reasonably accounts for the measured ratio in the entire energy range.

3.2.2. Anti-proton-induced double-ionization and the ratio. We present the calculated double-ionization cross section by incident anti-protons along with the observed data in

Table 5. Comparison between the calculated double-ionization cross section of He by anti-proton, σ (this work) and the selected observed data σ (Aarhus data).

Energy (keV)	σ (this work) (10^{-18} cm^2)	σ (Aarhus data[a]) (10^{-18} cm^2)
50.00	3.522	
53.90		2.011 ± 0.205
60.00	2.959	
67.10		1.923 ± 0.156
70.00	2.461	
80.00	2.226	
80.40		1.543 ± 0.139
90.00	1.956	
91.20		1.657 ± 0.145
100.00	1.837	
101.60		1.577 ± 0.123
200.00	0.877	
227.90		0.720 ± 0.039
270.10		0.696 ± 0.035
300.00	0.687	
400.00	0.491	
403.60		0.447 ± 0.023
500.00	0.363	
503.60		0.410 ± 0.021
600.00	0.296	
700.00	0.253	
800.00	0.221	
900.00	0.197	
1 000.00	0.170	
2 000.00	0.088	
3 000.00	0.060	
4 000.00	0.045	
5 000.00	0.037	
6 000.00	0.030	
7 000.00	0.025	
8 000.00	0.023	
9 000.00	0.020	
10 000.00	0.018	
30 000.00	0.006	
40 000.00	0.005	
50 000.00	0.004	

[a] Andersen *et al* (1987a, b 1989a, b), Hvelplund (1994).

the incident energy range of 40 keV–50 MeV in table 5 and have plotted them in figure 5. The calculation does account for the data in this large energy range and the observation that the double-ionization cross section by incident protons systematically lies lower than that by anti-protons in the energy range of 100–500 keV. The calculation predicts this trend to continue right up to 50 MeV. This is a consequence of the fact that the three terms in (9) have the same sign for the incident anti-proton case but not for the incident proton.

The calculated ratio of the double- to single-ionization cross section is presented and compared with experimental observation in table 6 and figure 6. The data cover a very large energy range, from a few tens of keV–20 MeV. The theoretical calculation can satisfactorily account for the data essentially in the entire energy range.

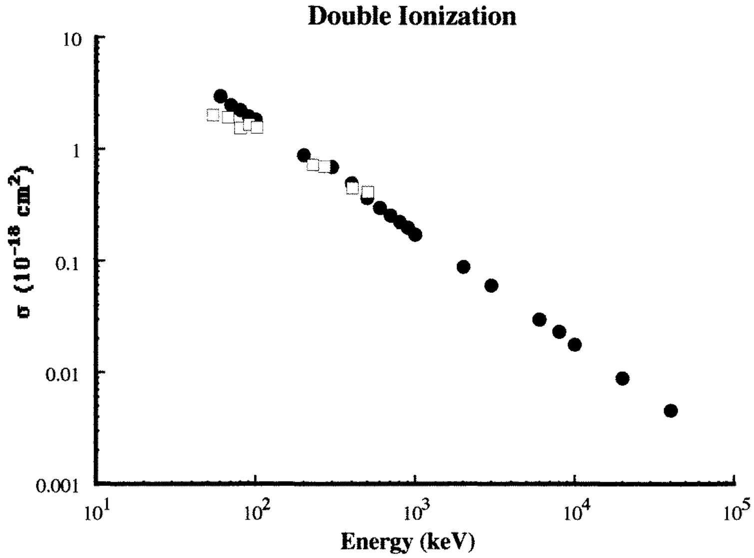

Figure 5. Calculated double-ionization cross section of He by anti-protons, denoted by ●, is compared with the selected data: □, Aarhus group data (Andersen *et al* 1987a, b, Hvelplund *et al* 1994).

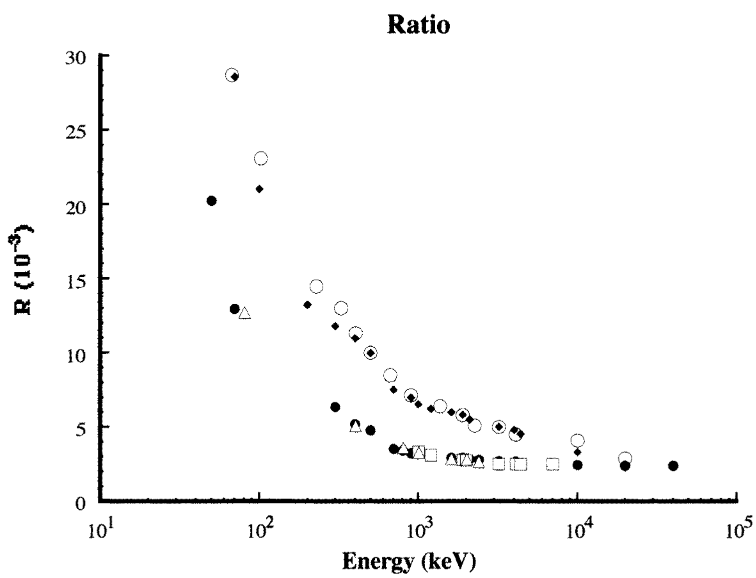

Figure 6. Calculated ratio of double- to single-ionization cross sections for incident protons, (●, this work (p^+)) and incident anti-protons, (♦, this work (p^-)) are compared with the corresponding incident proton data (△, Shah and Gilbody 1985, Shah *et al* 1989) and incident anti-proton data (○, Aarhus group (p^-)).

3.2.3. General discussion. In section 3.1.3, the possibility of resonances or the formation of a virtual (anti-proton–He) system has been raised. Such a physical situation would also influence the double-ionization cross section of He by anti-proton and hence the ratio. This

Table 6. Comparison between the calculated ratio of double- to single-ionization of He by proton and anti-proton noted in columns 2 and 5, respectively, and the corresponding data for incident proton and incident anti-proton noted in columns 3, 4 and 6, respectively.

Energy (keV)	This work (p^+) ($\times 10^{-3}$)	Aarhus group[a] (p^+) ($\times 10^{-3}$)	Shah[b] (p^+) ($\times 10^{-3}$)	This work (p^-) ($\times 10^{-3}$)	Aarhus group[a] (p^-) ($\times 10^{-3}$)
50.00	20.230				
67.10					28.70 ± 2.30
70.00				28.591	
80.67			12.70 ± 1.20		
100.00	10.104			21.023	
102.00					23.10 ± 1.10
200.00				13.225	
227.90					14.46 ± 0.78
300.00	6.363			11.799	
326.30					13.00 ± 0.66
400.00	5.279			10.987	
403.18	5.207		5.36 ± 0.28	10.529	
403.60					11.32 ± 0.58
500.00	4.776			9.997	10.00 ± 0.60
503.97	4.715		4.65 ± 0.27	8.546	
667.00					8.50 ± 0.30
700.00	3.523			7.516	
800.00	3.428			7.245	
806.35	3.414		3.60 ± 0.20	7.207	
900.00	3.234			6.995	7.15 ± 0.25
1 000.00	3.182	3.22 ± 0.10		6.532	
1 007.90	3.163		3.29 ± 0.16	6.524	
1 200.00	2.964	3.12 ± 0.20		6.231	
1 370.00					6.40 ± 0.19
1 612.70	2.926		2.86 ± 0.21	6.002	
1 900.00	2.886	2.80 ± 0.20		5.830	5.80 ± 0.25
2 000.00	2.842	2.76 ± 0.06		5.640	
2 015.90	2.833		2.82 ± 0.26	5.621	
2 100.00	2.820			5.492	
2 260.00					5.10 ± 0.41
2 398.90	2.819		2.66 ± 0.18	5.364	
3 000.00	2.776	2.64 ± 0.14		5.136	
3 200.00	2.693	2.50 ± 0.20		5.004	5.00 ± 0.25
4 100.00	2.647	2.50 ± 0.15		4.705	4.50 ± 0.25
4 400.00	2.600	2.50 ± 0.10		4.549	
7 000.00	2.523	2.51 ± 0.07		3.858	
10 000.00	2.515	2.49 ± 0.10		3.323	4.10 ± 0.41
20 000.00	2.450			2.302	2.90 ± 0.20

[a] Selected data of Andersen *et al* (1987a, b, 1989a, b), Hvelplund *et al* (1994).
[b] Selected data of Shah and Gilbody (1985), Shah *et al* (1989).

process is estimated to occur at a few tens of keV. Kimura *et al* (1994) have incorporated such processes in their calculation of the ratio of incident energies below 50 keV and found them to be important. This process is absent for the incident proton for which, on the other hand, the charge transfer channel becomes available. Kimura *et al* (1994) calculations seem to explain the observed difference in R for the two cases at energies below 50 keV. Incorporation of such phenomena is beyond the scope of our investigation which is, therefore, restricted to incident energy greater than about 80 keV. At very low incident energy, the Fermi and Teller (1947) effect, might also significantly influence the double-ionization cross section of He by anti-proton.

Satisfactory explanation of the observed data for the double- and single-ionizations and their ratios for the incident energies above 80 keV indicates that the coupled-channel method is a suitable one for describing the ionization process at incident energies significantly higher than the ionization thresholds. Because the perturbed potential (9) is different for the double-ionization cross section for the two cases, one theoretically predicts that the cross section for incident anti-proton will be higher than that by incident proton at incident energies greater than those used in current experiments. It would be interesting to verify this.

Theoretically, in the calculations of ionization cross sections by electron impact, the perturbation should be the same as the one for the anti-proton case. It would have, however, the additional complication of incorporating the Pauli principle which is important at lower incident energy (Malik and Trefftz 1961, Trefftz 1963). For He target, the effect of the Pauli principle on the cross section may not be critical for incident-electron energies greater than 10 keV and the situation is then similar to that for incident anti-proton, except for the difference in masses. Hence, the energy dependence of the ratio should be qualitatively the same in both cases, which is indeed the case experimentally (Stephan *et al* 1980, Andersen *et al* 1987).

Within the framework of the 2cPWBA, the alpha-induced ionization cross section should be similar to that of the incident proton, except that the masses of two projectiles are different. This difference would cause the key features of the energy dependence of the cross sections such as the maxima to occur at different energies in the two cases but the general pattern should be the same. This seems to be the case experimentally (Shah *et al* 1989).

4. Conclusion

The observed single- and double-ionization cross sections as well as their ratio for proton- and anti-proton-induced ionization of He can reasonably be accounted for in the 2cPWBA for the incident-energy range of a few tens of keV to a few tens of MeV. The 2cPWBA is essentially the Born approximation that includes proper interactions as perturbation if hydrogen-like electronic orbitals are used in the final channel. The calculation indicates that the proton and anti-proton induced cross sections for the single- and the double-ionization are different in the MeV region. Below a few tens of keV other factors such as intermediate channels and explicit inclusion of resonances might have to be considered.

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