Physica 79B (1975) 292–302
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ANGULAR DISTRIBUTION OF ELECTRONS EJECTED BY CHARGED PARTICLES

IV. COMBINED CLASSICAL AND QUANTUM-MECHANICAL TREATMENT

L. G. J. BOESTEN
Fysisch Laboratorium der Rijksuniversiteit Utrecht, Utrecht, The Netherlands
and
T. F. M. BONSEN
Moller Instituut, Tilburg, The Netherlands

Received 28 November 1974

Angular distributions of electrons ejected from helium by 100 and 300 keV protons have been calculated by a method which is a comination of the classical three-body collision theory and the quantum-mechanical Born approximation. The results of this theory have been compared with the corresponding experimental data and results of the Born and the classical three-body collision theories. The results of the combined method are in close agreement with the experimental data over the whole range of the ejection angles.

1. Introduction

The energy and angular distribution of electrons ejected from helium by proton impact has been measured by Rudd *et al.* [1]), Stolterfoht[2]) and Toburen[3]). These measurements have been compared with various theoretical predictions of the plane-wave Born approximation and the binary-encounter theory. Rudd *et al.* used the Born approximation to describe the ionization of atomic hydrogen and scaled the results with respect to the binding energy of helium. Madison[4]) also used the Born approximation to describe ionization of helium using bound and continuum electron wavefunctions obtained from a Hartree–Fock potential. Bonsen and Vriens[5]) performed calculations with the binary-encounter theory in which five different wavefunctions were used. All these approximations however failed to describe correctly the ejection of electrons with moderate energy in the forward direction. The binary-encounter theory, as all classical theories, could not describe ejection of electrons in the backward direction. Oldham[6]) suggested that the discrepancy between experimental and theoretical results for forward ejection might originate from a final-state interaction between the outgoing electron and the proton. An extension of the Born calculations for atomic hydrogen was made by Salin^{7}), who took into account the interaction of the ejected electron and the scattered proton in an impact-parameter treatment. An approximate solution of the Faddeev equations for the three-particle final state was given by Macek^{8}). In contrast to the quantum-mechanical approximations, Bonsen and Banks^{9}) performed calculations using the classical three-body collision theory, developed by Abrines and Percival^{10}). The (quantum-mechanical) calculations by Rudd *et al.*^{1}), Madison^{4}) and Salin^{7}) failed to describe the low-energy ejection in the forward direction, but they explained very well the ejection in the backward direction. The calculations by Macek^{8}) give results which are too large for ejection of electrons in the forward direction compared with the experiment. Bonsen and Banks^{9}) showed that for not too large angles of ejection (50° for 100 keV and 70° for 300 keV protons) their classical cross sections agree very well with the experimental values.

From the comparison of all these calculations with the measurements, the following remarks can be made:

i) collisions resulting in large energy and momentum transfers are generally close collisions and can be described with classical theories. To describe the ejection of electrons with low energy in the forward direction a three-body collision model is necessary.

ii) Backward ejection, which is generally a result of the reflection of the electron with positive total energy from the potential wall of the field of the nucleus, and occurring when momentum transfer is small, can only be described in a quantum-mechanical model (see ref. 11).

From these conclusions, it seems convenient to define a limit q_c of momentum transfer in such a way that for a momentum transfer larger than q_c the collision can be described with the classical three-body collision theory while for a momentum transfer smaller than q_c the Born approximation is applied.

2. Theory

2.1. *The Born approximation*

In the Born approximation the cross section for ionization of hydrogen atoms by charged particles ejecting the atomic electron with an energy between E and $E + \Delta E$ into the solid angle $\Delta\omega = \sin\theta\,\Delta\theta\,\Delta\phi$ can be written as:

$$\sigma(E,\theta) = \frac{8\pi^3 M^2 Z^2 e^4}{h^4 k^2} \int_{q_{\min}}^{\infty} q\,\mathrm{d}q \left| \int\!\!\int \frac{\exp(\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{R})}{|\boldsymbol{R}-\boldsymbol{r}|} \psi_{\kappa}^{*}\,\psi_i\,\mathrm{d}\boldsymbol{R}\,\mathrm{d}\boldsymbol{r} \right|^2 \qquad (1)$$

with $q_{\min} = (4\pi^2 M/kh^2)(E + U_{\mathrm{H}})$. In this formula q is the momentum change, M the mass, Z the charge, k the original momentum of the incident proton, R and r are the position vectors of the incident proton and the atomic electron with respect to the atomic nucleus respectively and ψ_{k} and ψ_i are the wavefunctions for the final and the initial states of the atomic electrons. E and U_{H} are the energy of the ejected electron and the binding energy, respectively. In the scaled Born approximation the differential cross sections for helium can be derived from the results for hydrogen by scaling[1])

$$\sigma(E,E_{\mathrm{pr}}, U_{\mathrm{He}}, n) = n\left(\frac{U_{\mathrm{H}}}{U_{\mathrm{He}}}\right)^3 \sigma\left(\frac{U_{\mathrm{H}}}{U_{\mathrm{He}}}\,E,\ \frac{U_{\mathrm{H}}}{U_{\mathrm{He}}}\,E_{\mathrm{pr}},\ U_{\mathrm{H}}, 1\right), \tag{2}$$

where E_{pr} is the energy of the incoming proton, E is the energy of the ejected electron, U_{H} and U_{He} are the ionization energies of hydrogen, and helium respectively, n is the number of the atomic electrons ($n = 2$ for He).

2.2. *The classical three-particle collision theory*

We have calculated the differential cross sections $\sigma(E,\theta)$ using the same method as described by Bonsen and Banks[9]). In the case of ionization of helium, an additional approximation has to be made in the classical three-body theory. The two electrons will be considered as independent scattering centres. Under this assumption the p–He collision can be described by two independent p–H collisions. The binding energy has to be chosen equal to the ionization energy of He. If we assume that no ionization takes place for impact parameters larger than $b_{\max}$, the double differential cross section $\sigma(E,\theta)$ for ejection of the atomic electron in a direction between $\theta - \frac{1}{2}\Delta\theta$ and $\theta + \frac{1}{2}\Delta\theta$ with respect to the direction of the incident protons, and with energy between $E - \frac{1}{2}\Delta E$ and $E + \frac{1}{2}\Delta E$, can be written as:

$$\sigma(E,\theta) = \frac{n(E,\theta)}{N_{\mathrm{tot}}\sin\theta\,\Delta\theta\,\Delta E}\cdot b_{\max}^2\,, \tag{3}$$

where N_{tot} is the total number of calculated collisions and $n(E,\theta)$ is the number of collisions, which have resulted in ejection of the atomic electron in direction θ and with energy E.

2.3. *The combined method*

As we have described previously, it is convenient to distinguish between collisions which result in large momentum transfer and the collisions which result in small momentum transfer. To describe these latter collisions, at least for ejection of the electron in the backward direction, a quantum-mechanical model is necessary. Therefore, we introduce a limit q_c for the momentum transfer so that for momentum transfer larger than q_c the collision can be described with the classical three-particle theory and for momentum transfer smaller than q_c with the Born approximation. Then we have for the double differential cross section the following expresion:

$$\sigma(E,\theta) = \frac{8\pi^3 M^2 Z^2 e^4}{h^4 k^2} \int_{q_{\min}}^{q_c} q\,\mathrm{d}q \left| \iint \frac{\exp(\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{R})}{|\boldsymbol{R}-\boldsymbol{r}|} \psi_K^* \psi_\mathrm{i}\,\mathrm{d}\boldsymbol{R}\mathrm{d}\boldsymbol{r} \right|^2 + \frac{n(E,\theta,q>q_c)}{N_{\mathrm{tot}} \sin\theta\,\Delta\theta\,\Delta E}\, b^2_{\max}. \tag{4}$$

To define an appropriate value for the momentum transfer q_c, Boesten *et al.*[13]) have calculated the generalized oscillator strengths for ionization of helium by proton impact, using the classical three-body collision theory. They have calculated these generalized oscillator strengths $f_E(q)$ as a function of the momentum change of the atomic electron. From these calculations the following conclusions can be made:

i) For small momentum changes ($q^2 < \sim 1-2$ a.u.) only quantum-mechanical theories can be used. All classical approximations fail to give the correct optical limit $f_E(0)$.

ii) For intermediate momentum changes ($\sim 1-2 < q^2 < \sim 15$ a.u.) the classical generalized oscillator strengths are larger than the oscillator strengths calculated with the Born and the binary-encounter approximations. In this region the three-particle interaction is important and gives a large contribution to the differential cross section $\sigma(E,q)$. Therefore, in this range the classical three-body collision theory gives more realistic cross sections than the Born approximation and the binary-encounter theory do.

iii) For large momentum transfer ($q^2 > \sim 15$ a.u.) the classical three-body collision theory, the binary-encounter and the Born approximations give the same generalized oscillator strengths. So, all collisions resulting in large momentum transfer can be described very well with classical approximations.

From these results we have concluded that the cutoff value of the momentum change q_c^2 must lie between 1 and 2 a.u. In our combined approximation, we have taken q_c equal to 1.22 ($q_c^2 = 1.5$). It is evident now that in the combined approximation the quantum-mechanical effects, which can give ionization with momentum change larger than q_c, are not included. Furthermore, in the Born approximation a minimum momentum transfer to the atomic electron is necessary, to eject this electron with a certain energy. So, the cutoff value q_c causes the contribution of the Born approximation to the differential and total cross sections to be significant up to a certain energy of the ejected electrons.

3. Results

3.1. *Double differential cross sections*

We have calculated the cross section $\sigma(E,\theta)$ and compared our results with the corresponding experimental results of Rudd *et al.*[1]). For 100 keV proton impact on helium the results are given in figs. 1 and 2. In fig. 1 we have presented the results for an ejection angle of 10 deg. In this figure we separately give the contribution to the double differential cross section $\sigma(E,\theta)$ due to the Born approximation (full line) and that due to the classical three-body collision theory (open squares). The contribution to the cross section from the Born approximation is restricted to ejection energies smaller than about 65 eV. For ejection energies larger than 65 eV there is only the contribution of the classical three-body collision theory. The results of the combined treatment are given by black squares.

The results for 30, 70 and 110 deg. ejection are presented in fig. 2. For 10 and 30 deg. ejection the agreement with the experimental results is extremely good. For larger ejection angles the agreement between the calculated and the experimental results becomes less good for ejection energies larger than 50 eV, due to the fact that the quantum-mechanical collisions are not, or not sufficiently, included for this range of ejection energies. From these results it is clear that there does not exist a sharp cutoff between the quantum-mechanical and the classical collisions. This means that it is impossible to describe the double differential cross sections for all ejection angles and energies with the combined treatment by introducing only one cutoff value q_c for the momentum transfer.

The results for 300 keV proton impact in helium are presented in fig. 3 together with the experimental results of Rudd *et al.*[1]). For 20 deg. ejection the cross section is given in the upper part of the figure. The agreement with experiment is very good, which is also the case for 50 deg. ejection. There exists also a very good agreement with experiment for 110 deg. ejection, for ejection energies smaller than about 80 eV. For 300 keV proton impact the contribution of the Born approximation to the cross section is restricted to the region below about 130 eV. So the combined method underestimates the double differential cross sections compared with experiment and with the Born approximation itself, for ejection angles larger than 90 deg., for large ejection energies (50 eV for

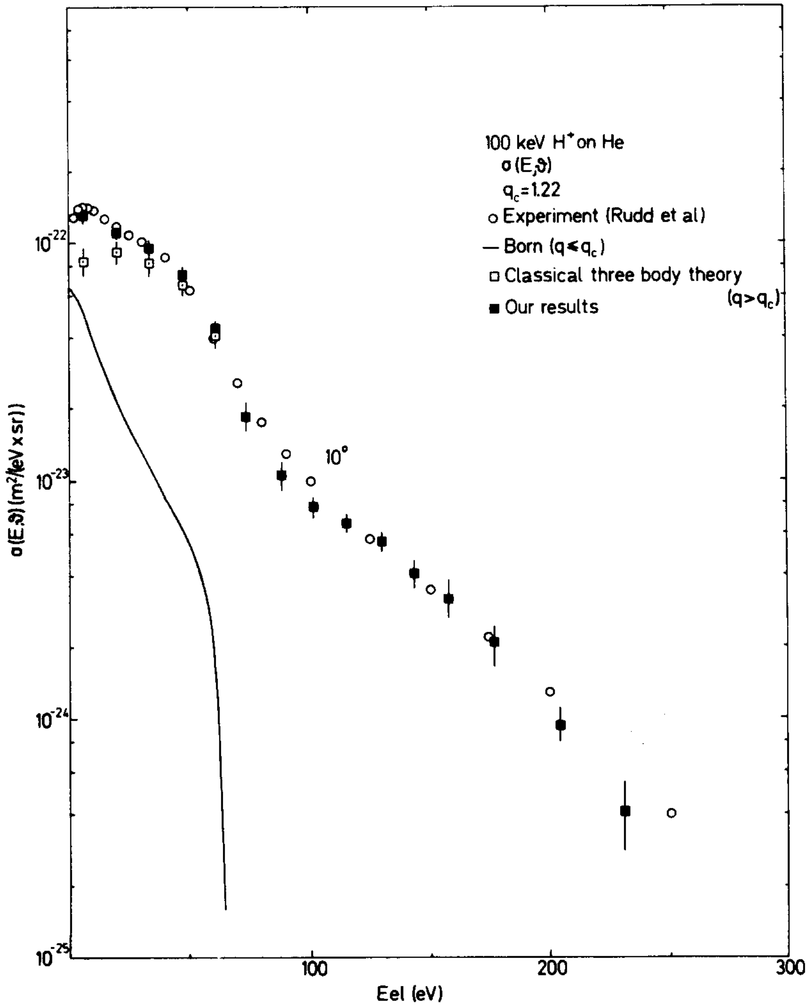

Fig. 1. Energy distribution of electrons ejected from helium under an angle of 10 deg. with respect to a 100 keV proton impact beam.

100 keV proton impact; 100 eV for 300 keV proton impact). In this region, however, the cross sections are very small and the errors in the experimental data are very large.

3.2. *Single differential cross sections*

In fig. 4 the single differential cross sections $\sigma(\theta)$ are presented and compared with the experimental results of Rudd *et al.*[1]), the Born calculations of Rudd *et al.*[1]) and the classical results of Bonsen and

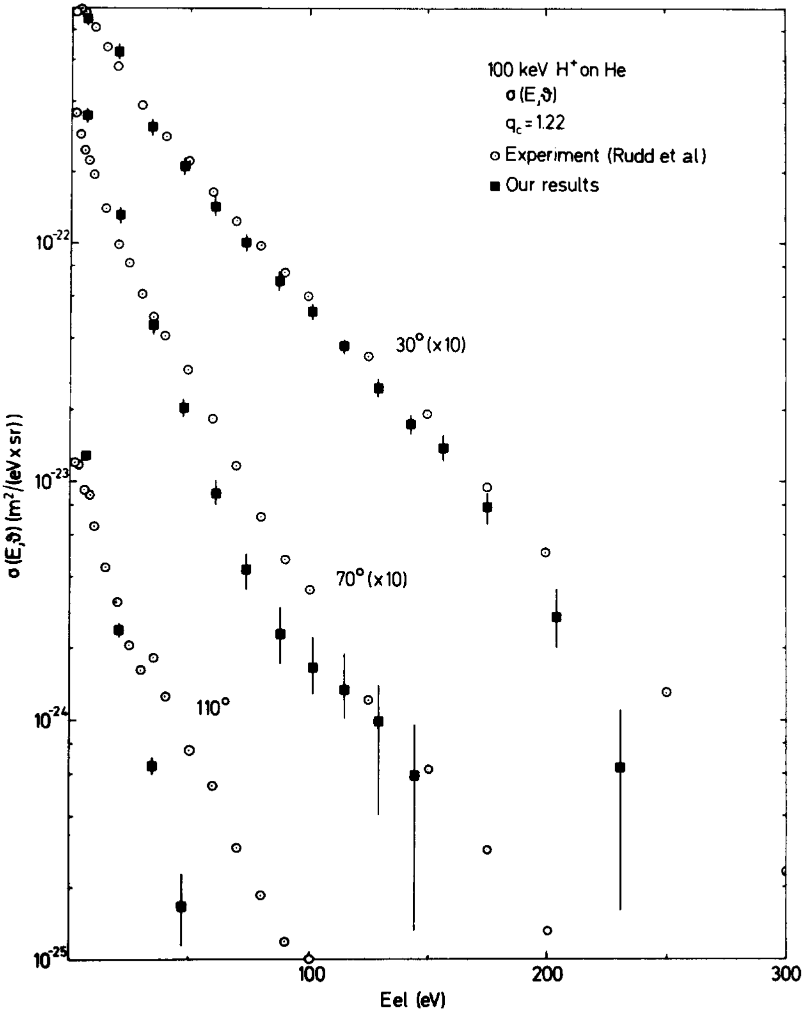

Fig. 2. Energy distribution of electrons ejected by 100 keV protons from helium at various angles. The set of data for 30 and 70 deg. ejection are multiplied by a factor of 10.

and Banks[9]). From these figures it is clear that the angular distribution calculated with the combined method is in very close agreement with experiment in the forward direction. But also for ejection angles larger than 90 deg. the agreement with the experiment is very good, especially in the case of 300 keV proton impact. In the case of 100 keV proton impact the discrepancy between calculated and experimental results is about 25%. This discrepancy is mainly due to the fact that for very small ejection energies ($E_{\mathrm{el}} < 2$ eV) the Born results are twice as large as the corresponding experimental results.

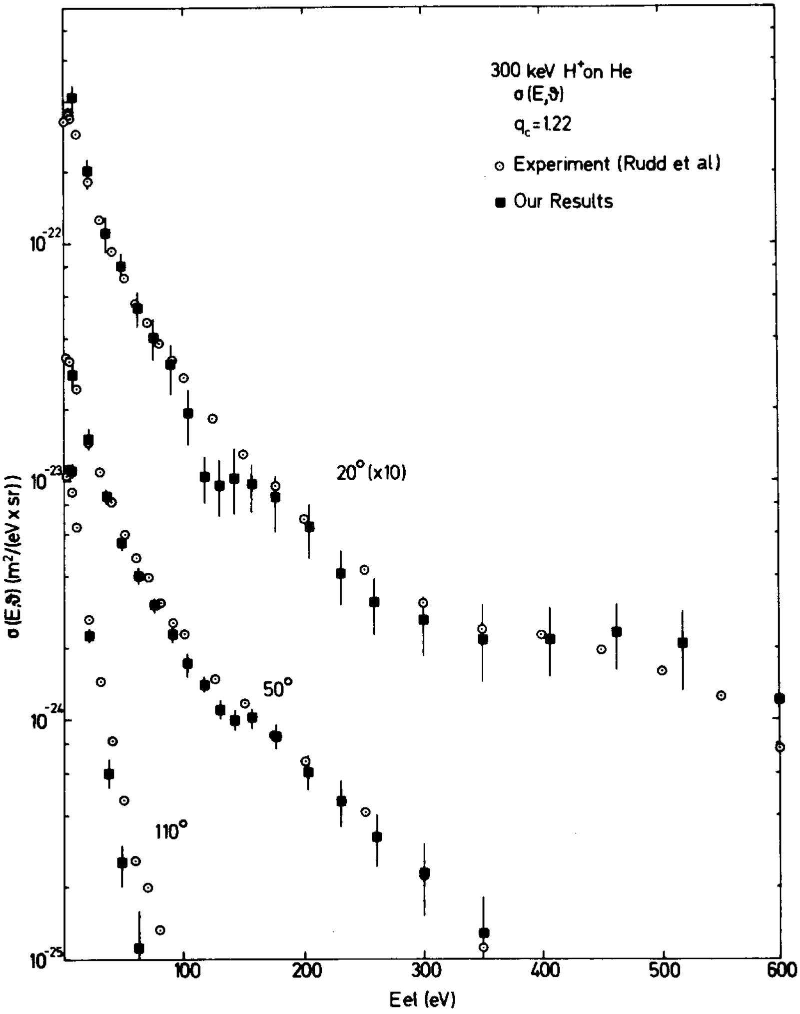

Fig. 3. Energy distribution of electrons ejected by 300 keVprotons from helium at various angles. The data for 20 deg. ejection are multiplied by a factor of 10.

3.3. *Total ionization cross sections*

In table I the total cross sections, calculated with the combined method, are presented for both incident energies and compared with previous results. It can be seen that the results, calculated with the combined method, are in very close agreement with the experimental results. For 100 keV proton impact the difference is only about 3.5%. The difference for 300 keV proton impact is about 8%. These differences are mainly caused by the ejection of electrons in the forward direction with very small

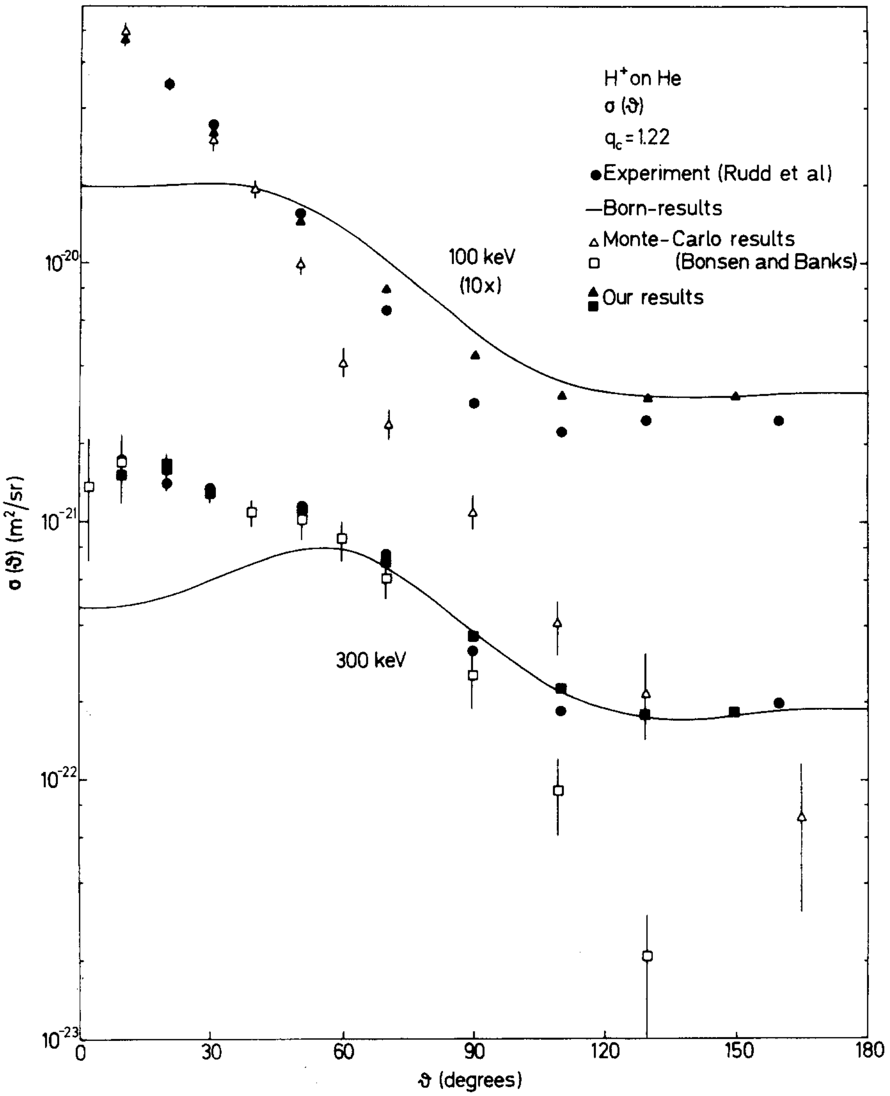

Fig. 4. Angular distribution of electrons ejected from helium by 100 and 300 keV protons respectively. The data for 100 keV are multiplied by a factor of 10.

ejection angles ($\theta < 10$ deg.). Due to the very small solid angle in these cases the statistical errors can be very large.

3.4. *Cross section dependence on the cutoff value of momentum transfer*

In the present results we have chosen the cutoff value of momentum transfer q_c equal to 1.22. To check the influence of this cutoff value we have also performed calculations for $q_c = 1.00$ and $q_c = 1.41$ ($q_c^2 = 1$ or 2,

TABLE I
Total ionization cross sections for ionization of helium by protons. All cross sections are given in units of 10^{-21} m^2

E_p (keV)	Rudd *et al.* (experiment)	Born (quantum-mechanical)	Bonsen *et al.* (classical)	Our results
100	11.9	11.0	9.25 ± 0.25	11.48 ± 0.25
300	7.13	5.47	5.44 ± 0.25	6.53 ± 0.25

respectively). For $q_c = 1$ the contribution of the quantum-mechanical Born approximation is restricted to ejection energies of 48 eV and 100 eV for 100 and 300 keV proton impact respectively. For $q_c = 1.41$ these values are 79 and 154 eV respectively.

The choice of the cut-off value q_c is only important for the double differential cross section $\sigma(E,\theta)$. A larger value of q_c will give a larger energy range where the Born approximation contributes to $\sigma(E,\theta)$. Simultaneously, the contribution of the classical three-particle collision theory will be reduced.

In the single differential cross sections the backward ejection is not affected by the value of q_c. For small ejection energies there is only a shift in the cross section $\sigma(\theta)$ within a few percent. Therefore, the choice of q_c (between 1 and 1.41) is not critical for total and single differential cross sections.

4. Conclusions

The combined method describes very well the angular and energy distribution of electrons ejected by protons from helium for small and intermediate ejection angles, for all ejection energies. For large ejection angles ($\theta > 90$ deg.) the combined method gives good results for small ejection energies.

The angular distribution of electrons ejected from helium by protons is described very well by the combined method. The agreement of the total ionization cross section with experiment is within 4% for 100 keV proton impact and within 8% for 300 keV proton impact.

Acknowledgements

We are indebted to Professor I. C. Percival for providing us with the computer programme (Monte-Carlo calculation) to do the classical three-body collision calculations.

The work of L. G. J. Boesten is part of the research programme of the Foundation for Fundamental Research on Matter (F.O.M.) and was financially supported by the Netherlands Organization for the Advancement of Pure Research (Z.W.O.).

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