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Multiple Scattering Calculation for Ionisation of Helium Atoms by Electrons at Intermediate Energies

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Abstract

The triple differential cross section for electron impact ionisation of helium atoms has been calculated in the coplanar asymmetric geometry following the multiple scattering approach of Das. The method has already been successfully employed to describe the electron impact ionisation problem for the hydrogen atom. Here the impact energy of the incident electron is taken to be 150 and 250 eV in an intermediate energy range where there are still some discrepancies between theory and experiment. Present results are compared with the available experimental data and with two of the most recent calculations in some cases, and are found to be in reasonable accord with experiment, particularly in the binary peak region. The present calculation for 250 eV incident energy reproduces the experimental results in some cases better than other theories.

1. Introduction

There has been increasing theoretical interest in the past few decades in the study of ionisation of atoms by electron impact. Apart from their importance in applications in other areas such as plasma physics or astrophysics, these studies are also interesting from a purely theoretical point of view as they provide a testing ground for various approximation schemes for many-body problems and also help us in understanding the basic collision dynamics. The complications associated with the many-body nature of the systems, and the subtlety introduced due to the infinite range of the Coulomb interactions involved, make atomic ionisation problems very interesting and challenging.

The most detailed information about the ionisation process is obtained from an analysis of the triple differential cross section (TDCS) measured in (e, 2e) coincidence experiments. The TDCS is a measure of the probability that in an (e, 2e) reaction an incident electron of energy $E_{\rm i}$ and momentum $\boldsymbol{p}_{\rm i}$, on collision with the target, will produce two outgoing electrons of energies E_1 and E_2 and momenta $\boldsymbol{p}_1$ and $\boldsymbol{p}_2$, emitted into the differential elements of the solid angles Ω_1 and Ω_2, centred about the directions (θ_1, ϕ_1) and (θ_2, ϕ_2) respectively. In this paper, our attention is confined to the calculation of the TDCS for electron impact ionisation of helium atoms in the Ehrhardt-type coplanar geometry characterised by small momentum transfer. It may be noted here that this type of kinematical situation provides a sensitive testing ground for the analysis of a theoretical

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model and also that the majority of ionisation events at intermediate and high energies of incidence occur at small momentum transfer.

The electron impact ionisation cross section (TDCS) of helium has been studied extensively within the framework of the first Born approximation (see Jacobs 1974; Geltman 1974; Robb *et al.* 1975; Franz and Klar 1986). It has been established from these studies that the first Born approximation is inadequate in explaining the characteristic features of the TDCS, even for impact energies as high as ten to a hundred times the ionisation potential. Subsequently, attempts have been made to include higher-order effects in various ways (see Byron *et al.* 1982, 1986; Ehrhardt *et al.* 1982; Curran and Walters 1987; Curran *et al.* 1991; Madison *et al.* 1977; Bransden *et al.* 1978; see also Ehrhardt *et al.* 1986).

One source of error in these calculations is the inaccurate treatment of the correlation between the electrons, particularly in the final channel. Brauner *et al.* (1989) tried to take into account exactly this correlation in the final channel in their wavefunction for the final channel scattering state, which is exact in the asymptotic limit. They used it in the study of ionisation of hydrogen atoms by electron impact. However, in their calculations short-range forces were not treated appropriately and as a consequence, though their results for the TDCS are qualitatively excellent, quantitatively there are discrepancies between their predictions and experiment. Later, Franz and Altick (1992) considered an approximation which is a generalisation of the approach of Brauner *et al.* They applied a high-energy approximation to the correlation term and the scattered electron wavefunction of Brauner, and the effect of the distortion of the slow ejected electron due to the He^+ core was introduced through a phase shift in the partial wave expansion of its wavefunction. They obtained very good agreement with experiment above 250 eV, but in the region up to 250 eV there are some discrepancies. Very recently Jones *et al.* (1993) included this phase factor in the standard distorted-wave Born approximation and the resultant approximation scheme, which they termed the 3DWBA, turns out to give a very satisfactory representation of the experimental results. However, there are exceptions in some cases. Their TDCS results for $E_{\rm i} = 250$ eV, $E_1 = 10$ eV, $\theta_2 = 16°$ do not agree very well with the measured results. This may not be due to inaccuracies in the measurements, as the authors suggest, but may be an indication of the fact that their theory does not hold with sufficient accuracy for large momentum transfers.

Quantitatively, the results of the 3DWBA calculation are very similar to that of a calculation by Srivastava and Sharma (1988). This later calculation (CB2) is only an improved version of the second Born approximation. Although the results of this calculation are very good for high energies, say 400 eV, they are not fully satisfactory for lower energies. The CB2 results tend to underestimate the binary peaks at larger momentum transfer (see Figs 2 and 3 of Schlemmer *et al.* 1991 and also Figs 1 and 2 of the present paper).

Recently we used the multiple scattering formalism of Das (1990) in studies of ionisation of hydrogen atoms by electrons (see Das and Seal 1993*a*, 1993*b*). The TDCS results are seen to be satisfactory for the binary peak regions, particularly in the case of large momentum transfers. Here we have employed the same formalism in the study of the TDCS for the ionisation of helium atoms by electron impact for an intermediate energy range, with simple modifications being introduced wherever these appear necessary.

2. Theory

The multiple scattering formalism of Das, described in detail for the ionisation problem for hydrogen atoms by Das and Seal (1993a), needs little modification for application to the ionisation problem for helium atoms. The (direct) T-matrix element for ionisation of helium atoms by electrons is given by

$$T_{\rm d} = \langle \Psi_{\rm f}^{(-)}(\boldsymbol{r}_1, \boldsymbol{r}_2, \boldsymbol{r}_3)|V_{\rm i}(\boldsymbol{r}_1, \boldsymbol{r}_2, \boldsymbol{r}_3)|\Phi_{\rm i}(\boldsymbol{r}_1, \boldsymbol{r}_2, \boldsymbol{r}_3)\rangle\,. \tag{1}$$

Here $\boldsymbol{r}_1, \boldsymbol{r}_3$ are the coordinates of the two electrons which in the initial channel are bound to form the helium atom, while $\boldsymbol{r}_2$ corresponds to the incident electron. Also, $\Phi_{\rm i}$ is the initial unperturbed state in the initial channel, $V_{\rm i}$ is the part of the interaction potential not included in the construction of the initial state, and $\Psi_{\rm f}^{(-)}$ is the final channel exact scattering state, which is the solution of the wave equation

$$\left(-\tfrac{1}{2}\nabla_1^2 - \tfrac{1}{2}\nabla_2^2 - \tfrac{1}{2}\nabla_3^2 + \frac{1}{r_{12}} + \frac{1}{r_{23}} - \frac{2}{r_1} - \frac{2}{r_2} - \frac{2}{r_3} - E_{\rm t}\right)\Psi_{\rm f}^{(-)} = 0\,. \tag{2}$$

Here $\Phi_{\rm i}(\boldsymbol{r}_1, \boldsymbol{r}_2, \boldsymbol{r}_3)$ is given by

$$\Phi_{\rm i}(\boldsymbol{r}_1, \boldsymbol{r}_2, \boldsymbol{r}_3) = (2\pi)^{-3/2}\, {\rm e}^{{\rm i}\boldsymbol{p}_{\rm i}\cdot\boldsymbol{r}_2}\, \phi(\boldsymbol{r}_1, \boldsymbol{r}_3)\,. \tag{3a}$$

where $\phi(\boldsymbol{r}_1, \boldsymbol{r}_3)$ is the ground-state wavefunction of the helium atom. For simplicity we use the wavefunction of Byron and Joachain (1966) given by

$$\phi(\boldsymbol{r}_1, \boldsymbol{r}_3) = \phi_0(\boldsymbol{r}_1)\, \phi_0(\boldsymbol{r}_3)\,, \tag{3b}$$

where

$$\phi_0(r) = (4\pi)^{-1/2}(A{\rm e}^{-\alpha r} + B{\rm e}^{-\beta r})\,, \tag{3c}$$

with parameters

$$\alpha = 1\cdot 41\,, \quad \beta = 2\cdot 61\,, \quad A = 2\cdot 60505\,, \quad B = 2\cdot 08144\,. \tag{3d}$$

In the final channel we have two outgoing electrons and a He^+ core. We approximate $\Psi_{\rm f}^{(-)}$ by

$$\Psi_{\rm f}^{(-)}(\boldsymbol{r}_1, \boldsymbol{r}_2, \boldsymbol{r}_3) = \phi_{\rm He^+}(\boldsymbol{r}_3)\, \Psi_{\rm f}^{(-)}(\boldsymbol{r}_1, \boldsymbol{r}_2)\,, \tag{4}$$

where

$$\phi_{\rm He^+}(\boldsymbol{r}_3) = (z_{\rm He}^3/\pi)^{1/2}\, {\rm e}^{-z_{\rm He} r_3}\,, \tag{5a}$$

and $\Psi_{\rm f}^{(-)}(\boldsymbol{r}_1, \boldsymbol{r}_2)$ is an exact solution of the two-particle Schrödinger equation

$$\left(-\tfrac{1}{2}\nabla_1^2 - \tfrac{1}{2}\nabla_2^2 - \frac{1}{r_1} - \frac{1}{r_2} + \frac{1}{r_{12}} - E\right)\Psi_{\rm f}^{(-)}(\boldsymbol{r}_1, \boldsymbol{r}_2) = 0\,. \tag{5b}$$

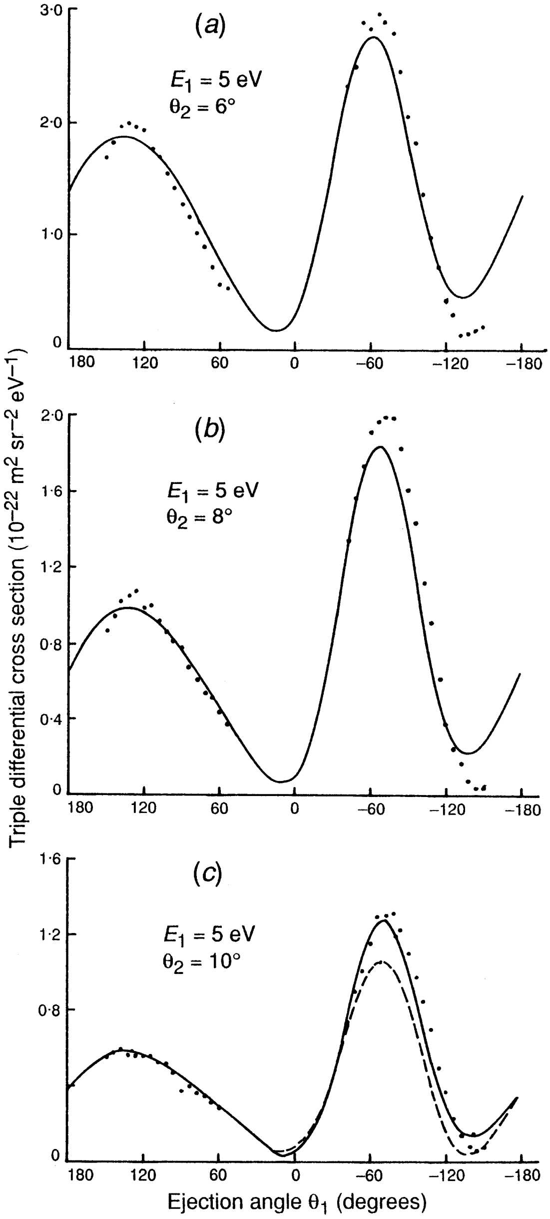

Fig. 1. Triple differential cross section versus ejection angle θ_1 for electron impact energy $E_{\rm i} = 250$ eV and for the values of E_1 and θ_2 indicated. Theory: continuous curve, present calculation; dashed curve, CB2 (Schlemmer *et al.* 1991). Experiment: Schlemmer *et al.* (1991).

So here the structure of the ion core is disregarded. The total energy of the system is given by

$$E_{\rm t} = \tfrac{1}{2}p_1^2 + \tfrac{1}{2}p_2^2 + \epsilon = E + \epsilon\,, \tag{5c}$$

where ϵ is the binding energy of the He^+ ground state and $\boldsymbol{p}_1, \boldsymbol{p}_2$ are the momenta of the two outgoing electrons, $\boldsymbol{p}_1$ being the momentum of the ejected electron.

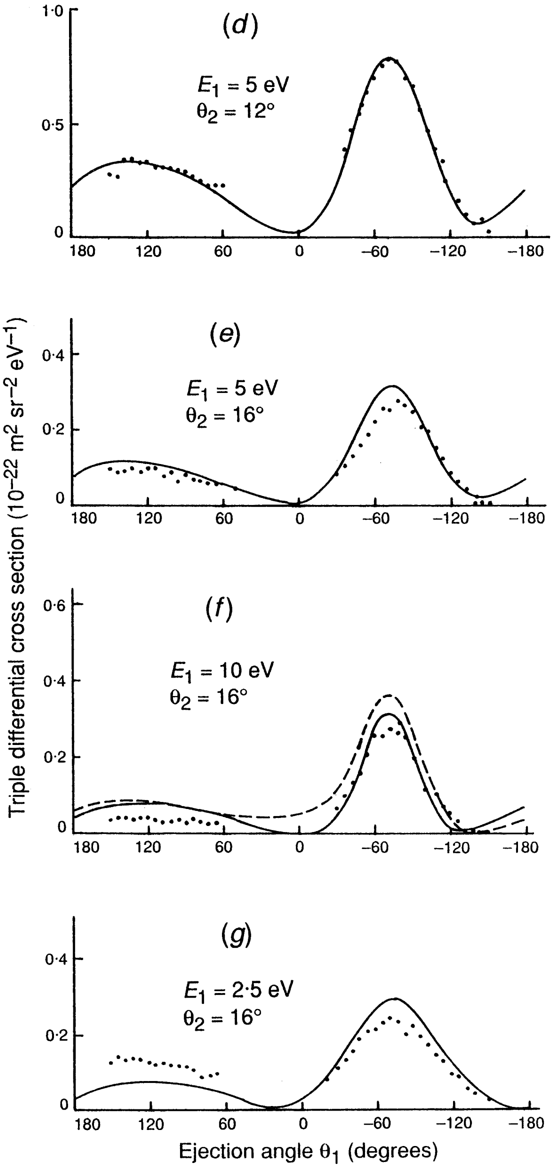

Fig. 1 *(continued)*

Now $\Psi_f^{(-)}$ is not exactly known. We use the approximate solution of Das and Seal (1993*a*) given by

$$\Psi_f^{(-)}(\boldsymbol{r}_1, \boldsymbol{r}_2) = N(\boldsymbol{p}_1, \boldsymbol{p}_2)\, \Phi_{\boldsymbol{p}_1, \boldsymbol{p}_2}^{(-)}(\boldsymbol{r}_1, \boldsymbol{r}_2)\,, \tag{6a}$$

where

$$\Phi_{\boldsymbol{p}_1, \boldsymbol{p}_2}^{(-)}(\boldsymbol{r}_1, \boldsymbol{r}_2) = \phi_{\boldsymbol{p}_1}^{(-)}(\boldsymbol{r}_1)\, e^{i\boldsymbol{p}_2 \cdot \boldsymbol{r}_2} + \phi_{\boldsymbol{p}_2}^{(-)}(\boldsymbol{r}_2)\, e^{i\boldsymbol{p}_1 \cdot \boldsymbol{r}_1}$$

$$+ \phi_{\boldsymbol{p}}^{(-)}(\boldsymbol{r})\, e^{i\boldsymbol{P} \cdot \boldsymbol{R}} - 2e^{i\boldsymbol{p}_1 \cdot \boldsymbol{r}_1 + i\boldsymbol{p}_2 \cdot \boldsymbol{r}_2}\,. \tag{6b}$$

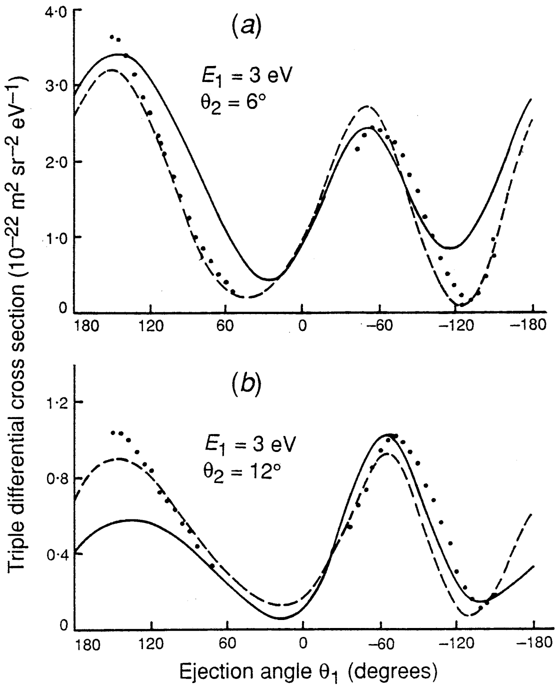

Fig. 2. Triple differential cross section versus ejection angle θ_1 for electron impact energy $E_i = 150$ eV and for the values of E_1 and θ_2 indicated. Theory: continuous curve, present calculation; dashed curve, 3DWBA (Jones *et al.* 1993); dash–dot curve, CB2 (Schlemmer *et al.* 1991). Experiment: Schlemmer *et al.* (1991).

Here $\boldsymbol{r} = \frac{1}{2}(\boldsymbol{r}_2 - \boldsymbol{r}_1)$, $\boldsymbol{R} = \frac{1}{2}(\boldsymbol{r}_2 + \boldsymbol{r}_1)$, $\boldsymbol{p} = \boldsymbol{p}_2 - \boldsymbol{p}_1$, $\boldsymbol{P} = \boldsymbol{p}_2 + \boldsymbol{p}_1$, and $\phi_{\boldsymbol{p}}$ is the Coulomb wavefunction

$$\phi_{\boldsymbol{p}}^{(-)}(\boldsymbol{r}) = \mathrm{e}^{\pi\alpha/2}\,\Gamma(1+\mathrm{i}\alpha)\mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}}\;{}_1F_1\big(-\mathrm{i}\alpha, 1, -\mathrm{i}(qr + \boldsymbol{q}\cdot\boldsymbol{r})\big)\,, \tag{6c}$$

with $\alpha = 1/p_1$ for $\boldsymbol{q} = \boldsymbol{p}_1$, $\alpha = 1/p_2$ for $\boldsymbol{q} = \boldsymbol{p}_2$ and $\alpha = -1/p$ for $\boldsymbol{q} = \boldsymbol{p}$.

The normalisation constant N is given by

$$|N(\boldsymbol{p}_1, \boldsymbol{p}_2)|^{-2} = 7 - 2(\lambda_1 + \lambda_2 + \lambda_3) - 2\left(\frac{1}{\lambda_1} + \frac{1}{\lambda_2} + \frac{1}{\lambda_3}\right) + \frac{\lambda_1}{\lambda_2} + \frac{\lambda_1}{\lambda_3} + \frac{\lambda_2}{\lambda_3} + \frac{\lambda_2}{\lambda_1} + \frac{\lambda_3}{\lambda_1} + \frac{\lambda_3}{\lambda_2}\,, \tag{6d}$$

where

$$\lambda_1 = \mathrm{e}^{\pi\alpha_1/2}\,\Gamma(1 - \mathrm{i}\alpha_1)\,, \qquad \alpha_1 = 1/p_1\,,$$

$$\lambda_2 = \mathrm{e}^{\pi\alpha_2/2}\,\Gamma(1 - \mathrm{i}\alpha_2)\,, \qquad \alpha_2 = 1/p_2\,,$$

$$\lambda_3 = \mathrm{e}^{\pi\alpha/2}\,\Gamma(1 - \mathrm{i}\alpha)\,, \qquad \alpha = -1/p\,.$$

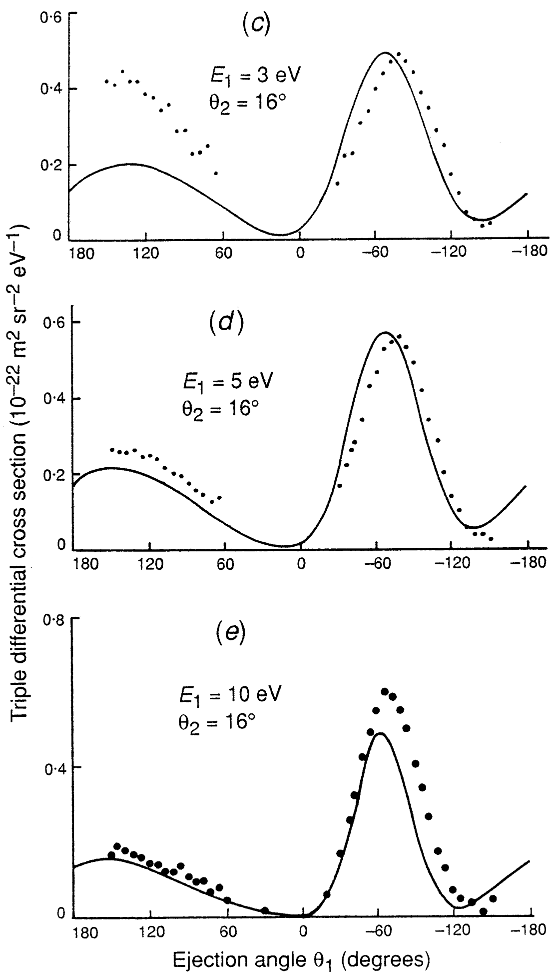

Fig. 2 *(continued)*

Detailed discussion on the normalisation constant N and the accuracy of the wavefunction is given in Das and Seal (1993*a*). In our present calculation for highly asymmetric geometry, the exchange amplitude and the capture amplitude are small and are neglected. The triple differential cross section is finally given by

$$\frac{\mathrm{d}^3\sigma}{\mathrm{d}\Omega_1\,\mathrm{d}\Omega_2\,\mathrm{d}E_1} = \frac{2}{(2\pi)^5}\,\frac{p_1 p_2}{p_\mathrm{i}}|T_\mathrm{d}|^2\,. \tag{7}$$

3. Results

Results of our calculation together with experimental results of Schlemmer *et al.* (1991) are presented in Figs 1 and 2. Fig. 1 displays the results for incident energy $E_\mathrm{i} = 250\,\mathrm{eV}$, while Fig. 2 corresponds to $E_\mathrm{i} = 150\,\mathrm{eV}$. Figs 1*a*–1*e* show the results for fixed ejection energy $E_1 = 5\,\mathrm{eV}$ and for scattering angles $\theta_2 = 6°$, 8°, 10°, 12° and 16° respectively, showing the cross section as the scattering angle continuously increases. Figs 1*e*–1*g* show the results for a fixed value of θ_2 equal to 16° and for E_1 values of 5, 10 and 2·5 eV respectively. From these figures it can be seen that the cross sections are in good agreement with the experimental data, particularly in the binary peak region for larger scattering angles. Small discrepancies which sometimes occur in these regions may perhaps be removed with the use of a more accurate wavefunction for the ground state of the helium atom. Cross sections in the recoil region are generally not very satisfactory. Similar features were also observed in our earlier studies on the ionisation of the hydrogen atom (Das and Seal 1993*a*).

Figs 2*a*–2*c* show the results for $E_i = 150$ eV, $E_1 = 3$ eV and θ_2 values equal to 6°, 12° and 16°; Figs 2*c*–2*e* are for θ_2 fixed at 16° and values of E_1 of 3, 5 and 10 eV respectively. These also show trends similar to those displayed in Fig. 1. However, in general, the results for $E_i = 150$ eV are seen to be somewhat less accurate compared with those for $E_i = 250$ eV. In several of the figures we have also presented results of the CB2 and 3DWBA calculations where available. These comparisons show that our results in the binary region are generally better than those of other calculations for larger scattering angles, while for smaller scattering angles CB2 and 3DWBA give a better reproduction of the experimental data. The present results for $E_i = 250$ eV, $E_1 = 10$ eV and $\theta_2 = 16°$ (Fig. 1*f*) support the experimental data, the accuracy of which was questioned by Jones *et al.* (1993).

4. Conclusions

Our multiple scattering calculation for the TDCS for ionisation of the helium atom gives results which are in satisfactory agreement with the experimental measurements in the case of the Ehrhardt asymmetric kinematic regime at intermediate energies. Results are excellent particularly for 250 eV incident energy in the binary peak region and especially for larger momentum transfer. This feature was also observed in our earlier ionisation studies on the hydrogen atom. Improved agreement with experiment may be achieved by using a more accurate wavefunction for the ground state of the helium atom. Besides, the exchange and capture processes, particularly the former, become significant for large momentum transfer collisions. Thus, for the calculation of cross sections at large momentum transfer, these amplitudes need to be considered properly. The measurements by Schlemmer *et al.* (1991) for $E_i = 250$ eV, $E_1 = 10$ eV and $\theta_2 = 16°$, about which doubts were expressed by Jones *et al.* (1993), are corroborated by our present calculation.

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