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$(e, 2e)$ triple differential cross section for ionization-excitation of helium

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Abstract. Simultaneous ionization and excitation of helium by electron impact is considered in an improved second Born approximation. The wave function of the low energy ejected electron is obtained in the field of residual He^+ ion in 2s-state. The calculation has been done for the process $e^- + He \rightarrow e^- + He^+(2s) + e^-$ in the coplanar asymmetric geometry with Hartree-Fock wave function of Byron and Joachain for the helium ground state and the results are compared with the absolute experimental data of Dupre *et al* [*J. Phys.* **B25**, 259 (1992)] at $\sim 5{\cdot}5$ keV incident energy. Our results are found to increase the ratio of the recoil peak to binary peak intensity by about 30% over the first Born results and thus to bring it closer to the experimental data.

Keywords. Excitation alongwith ionization; two active atomic electrons; second Born approximation.

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1. Introduction

Most of the $(e - 2e)$ studies have been confined to the ionizing processes which leave the residual positive ion in the ground state. However, the related process of simultaneous ionization and excitation of the target by the incoming electron has been studied very little. In this process, one electron is ejected and a second one is transferred to some available excited state of the residual ion. This process therefore provides an interesting link between the widely investigated single ionization $(e - 2e)$ area and the recently emerged double ionization $(e - 3e)$ area. It can proceed via two mechanisms:

(i) The shake-off (SO) mechanism which corresponds to single ionization followed by final state rearrangement.
(ii) The two-step (TS) mechanism in which the projectile interacts with both the atomic electrons.

Several studies have been carried out to probe the sensitivity of triple differential cross section (TDCS) to the initial and final state correlations. The process $e^- + He \rightarrow e^- + He^+(2s, 2p) + e^-$ has been investigated by Cook *et al* [1], Smith *et al* [2], Stefani *et al* [3], Avaldi *et al* [4] and Dupre *et al* [5] in high incident energy experiments. Calculations have been done in the framework of the first Born approximation with various prescriptions for obtaining ejected electron wave function [6–10]. The plane and distorted wave impulse approximations have also been used [2, 11, 12].

Recently a first order calculation with correlated Coulomb wave function of Brauner *et al* [13] has also been tried [14]. It is found that, in the asymmetric kinematics where the dynamics is more important, no single model is able to reproduce angular variation of TDCS at incident energies 645·4 eV, 1585·4 eV and ~5·5 keV where experimental data are available. However these calculations have indicated that the TDCS are not very sensitive to the $e-e$ correlations in the initial state, though they are important to allow collective ionization-excitation of the two target electrons in a first order model. On the other hand a proper description of the ejected electron which takes into account its interaction with the residual excited ion in $n=2$ state of larger spatial extent is crucial and is largely responsible for a larger recoil intensity and for an angular distribution whose shape is no longer made of the usual binary and recoil lobes. These features tend to vanish as the ejected electron energy increases.

In the present paper we investigate the role of (i) dynamic correlations in the continuum final state and (ii) two-step (TS) processes. The second order terms in the scattering amplitude are expected to be quite important up to certain high incident energies. The calculation has been done in the second Born approximation for asymmetric kinematics. A similar calculation was done by Saxena *et al* [15] at an incident energy of 600 eV and the results were compared with those for ionization without excitation. The present calculation differs from this attempt in the sense that the low energy ejected electron wave function is calculated in the static field of the residual ion. Earlier calculations have already underlined the importance of this feature. We have, for this study, considered the simple process $e^- + \text{He} \rightarrow e^- + \text{He}^+(2s) + e^-$ in the asymmetric kinematics at an incident energy of ~ 5·5 keV with the Hartree-Fock wave function of Byron and Joachain [16] for the helium ground state.

2. Calculation

The triple differential cross section (TDCS) for the ionization of helium may be expressed as

$$\frac{d^3\sigma}{d\Omega_a d\Omega_b dE_b} = \frac{k_a k_b}{k_0}|F|^2, \tag{1}$$

where F is the direct scattering amplitude and $\mathbf{k}_0$, $\mathbf{k}_a$ and $\mathbf{k}_b$ are the momenta of the incident, scattered and ejected electrons respectively. In the present improved second Born approximation the direct scattering amplitude may be expressed as

$$F_{CB2} = f_{CB1} + f_{CB2}, \tag{2}$$

where f_{CB1} and f_{CB2} are respectively the first and second order Born amplitudes. The amplitude f_{CB1} is given by

$$f_{CB1} = -\frac{1}{2\pi}\left\langle e^{i\mathbf{k}_a\cdot\mathbf{r}_0}\Phi_f(\mathbf{r}_1,\mathbf{r}_2)\left|\frac{1}{r_{01}}+\frac{1}{r_{02}}\right| e^{i\mathbf{k}_0\cdot\mathbf{r}_0}\Phi_0(\mathbf{r}_1,\mathbf{r}_2)\right\rangle. \tag{3}$$

Here $\mathbf{r}_0$, $\mathbf{r}_1$ and $\mathbf{r}_2$ are the position vectors of the incident and the two target electrons respectively, Φ_0 is the ground state wave function of helium atom which is taken to be the Hartree-Fock wave function of Byron and Joachain [16]:

$$\Phi_0(\mathbf{r}_1,\mathbf{r}_2) = u(\mathbf{r}_1)u(\mathbf{r}_2), \tag{4}$$

$$u(\mathbf{r}) = \sum_{i=1}^{2} \gamma_i e^{-\alpha_i r},$$

with

$$\alpha_1 = 1{\cdot}41, \quad \alpha_2 = 2{\cdot}61,$$

$$\gamma_1 = 0{\cdot}73485 \text{ and } \gamma_2 = 0{\cdot}58715.$$

The final state wave function Φ_f is taken to be the symmetrized product of the He^+ excited state (2s) wave function $v(\mathbf{r})$ for the bound electron with the continuum wave function $\psi^{(-)}_{\mathbf{k}_b}$ (orthogonalized to the ground state orbital $u(\mathbf{r})$) for the ejected electron:

$$\Phi_f(\mathbf{r}_1,\mathbf{r}_2) = \frac{1}{\sqrt{2}}[\psi^{(-)}_{\mathbf{k}_b}(\mathbf{r}_1)\, v(\mathbf{r}_2) + \psi^{(-)}_{\mathbf{k}_b}(\mathbf{r}_2)\, v(\mathbf{r}_1)], \tag{5}$$

$$v(\mathbf{r}) = \frac{1}{\sqrt{\pi}}(1-r)e^{-r}, \tag{6}$$

$$\psi^{(-)}_{\mathbf{k}_b}(\mathbf{r}) = \phi^{(-)}_{\mathbf{k}_b}(\mathbf{r}) - \langle u(\mathbf{r})|\phi^{(-)}_{\mathbf{k}_b}(\mathbf{r})\rangle u(\mathbf{r}). \tag{7}$$

Using (4)–(7) in (3) and integrating with respect to $\mathbf{r}_0$, we get

$$f_{\mathrm{CB1}} = -\frac{2^{3/2}}{K^2}\langle v|u\rangle[\langle\phi^{(-)}_{\mathbf{k}_b}(\mathbf{r})|e^{i\mathbf{K}\cdot\mathbf{r}}|u(\mathbf{r})\rangle - \langle u(\mathbf{r})|e^{i\mathbf{K}\cdot\mathbf{r}}|u(\mathbf{r})\rangle \langle\phi^{(-)}_{\mathbf{k}_b}(\mathbf{r})|u(\mathbf{r})\rangle], \tag{8}$$

where $\mathbf{K} = \mathbf{k}_0 - \mathbf{k}_a$. The wave function $\phi^{(-)}_{\mathbf{k}_b}(\mathbf{r})$ is written as

$$\phi^{(-)}_{\mathbf{k}_b}(\mathbf{r}) = \phi^{(-)}_{C,\mathbf{k}_b}(\mathbf{r}) + (\phi^{(-)}_{\mathbf{k}_b}(\mathbf{r}) - \phi^{(-)}_{C,\mathbf{k}_b}(\mathbf{r}))$$
$$= \phi^{(-)}_{C,\mathbf{k}_b}(\mathbf{r}) + \chi^{(-)}_{\mathbf{k}_b}(\mathbf{r}), \tag{9}$$

where $\phi^{(-)}_{C,\mathbf{k}_b}$ is the Coulomb wave function (corresponding to $Z = 1$) with appropriate boundary conditions

$$\phi^{(-)}_{C,\mathbf{k}_b} = e^{-\pi\eta/2}\Gamma(1-i\eta)e^{i\mathbf{k}_b\cdot\mathbf{r}}\,{}_1F_1(i\eta; 1, -ik_b r - i\mathbf{k}_b.\mathbf{r}), \tag{10}$$
$$\eta = -1/k_b.$$

The correction $\chi^{(-)}_{\mathbf{k}_b}(\mathbf{r}) \equiv (\phi^{(-)}_{\mathbf{k}_b}(\mathbf{r}) - \phi^{(-)}_{C,\mathbf{k}_b}(\mathbf{r}))$ is expressed in the partial wave form

$$\chi^{(-)}_{\mathbf{k}_b}(\mathbf{r}) = \sum_{\ell} i^{\ell}(2\ell+1)(e^{-i\delta_\ell}R_\ell(r) - e^{-i\delta^C_\ell}R^C_\ell(r))P_\ell(\hat{k}_b.\hat{r}). \tag{11}$$

Here, $R^C_\ell(r)$ is the ℓth Coulomb partial wave and δ^C_ℓ is the corresponding phase shift. The radial solution $R_\ell(r)$ and the phase shift δ_ℓ are obtained by solving the radial Schrödinger equation in the static field V_0 of He^+ ion:

$$V_0(r) = \int |v(\mathbf{r}')|^2 \left(\frac{2}{r} - \frac{1}{|\mathbf{r}'-\mathbf{r}|}\right) d\mathbf{r}'. \tag{12}$$

Using (9) and (11) in (8), one finally obtains

$$f_{CB1} = f_{B1} - \frac{2^{7/2}}{K^2}\pi C_1(0)\left[\sum_\ell (2\ell+1)P_\ell(\hat{K}.\hat{k}_b)D_\ell(K) - C_2(K)D_0(0)\right], \quad (13)$$

where

$$C_1(K) = \int v(\mathbf{r})u(\mathbf{r})e^{i\mathbf{k}.\mathbf{r}}d\mathbf{r}, \quad (14)$$

$$C_2(K) = \int u^2(\mathbf{r})e^{i\mathbf{K}.\mathbf{r}}d\mathbf{r} \quad (15)$$

and

$$D_\ell(K) = \int u(r)j_\ell(Kr)[e^{i\delta_\ell}R_\ell(r) - e^{i\delta_\ell^C}R_\ell^C(r)]r^2 dr. \quad (16)$$

The amplitude f_{B1}, is the usual first Born amplitude which is evaluated in the standard way [17, 16]. The second term in (13) represents the correction due to the improved choice, (9), in place of $\phi^{(-)}_{C,\mathbf{k}_b}(\mathbf{r})$ for the ejected electron wave function. The radial integral in (16) is evaluated numerically.

The second Born term f_{CB2} may be written as

$$f_{CB2} = \frac{1}{8\pi^4}\int d\mathbf{q}\frac{1}{q^2 - p^2 - i\varepsilon}M, \quad (17)$$

where

$$M = \frac{16\pi^2}{K_i^2 K_f^2}\langle\Phi_f(\mathbf{r}_1,\mathbf{r}_2)|(e^{-i\mathbf{K}_f.\mathbf{r}_1} + e^{-i\mathbf{K}_f.\mathbf{r}_2} - 2)$$
$$\times (e^{i\mathbf{K}_i.\mathbf{r}_1} + e^{i\mathbf{K}_i.\mathbf{r}_2} - 2)|\Phi_i(\mathbf{r}_1,\mathbf{r}_2)\rangle, \quad (18)$$

$p^2 = k_0^2 - 2\bar{\omega}, \mathbf{K}_i = \mathbf{k}_0 - \mathbf{q}$ and $\mathbf{K}_f = \mathbf{k}_a - \mathbf{q}$.

The excitation energies of the intermediate states have been approximated by an average excitation energy $\bar{\omega}$ and the sum over them carried out by using the closure property. We have taken $\bar{\omega}$ equal to the ionization energy plus the $n = 1$ to $n = 2$ excitation energy, $0{\cdot}9 + 1{\cdot}5 = 2{\cdot}4$ a.u. It is essentially a parameter. The results are, however, found to be not very sensitive to this choice. Using (4), (5), (14)–(16) in eq. (18), one obtains

$$M = \frac{16\sqrt{2}\pi^2}{K_i^2 K_f^2}[C_1(K_f)\langle\psi^{(-)}_{\mathbf{k}_b}(\mathbf{r}_1)|e^{i\mathbf{K}_i.\mathbf{r}_1}|u(\mathbf{r}_1)\rangle$$
$$+ C_1(K_i)\langle\psi^{(-)}_{\mathbf{k}_b}(\mathbf{r}_2)|e^{-i\mathbf{K}_f.\mathbf{r}_2}|u(\mathbf{r}_2)\rangle$$
$$+ C_1(0)\langle\psi^{(-)}_{\mathbf{k}_b}(\mathbf{r}_1)|e^{i\mathbf{K}.\mathbf{r}_1} - 2e^{i\mathbf{K}_i.\mathbf{r}_1} - 2e^{i\mathbf{K}_f.\mathbf{r}_1}|u(\mathbf{r}_1)\rangle], \quad (19)$$

which by using (7), (9) and (10) and the partial wave decomposition leads to

$$M = M_C + \frac{16\sqrt{2}\pi^2}{K_i^2 K_f^2}\Big[4\pi\sum_\ell(2\ell+1)\{C_1(0)D_\ell(K)P_\ell(\hat{K}.\hat{k}_b) + (C_1(K_f)$$
$$- 2C_1(0)D_\ell(K_i)P_\ell(\hat{K}_i.\hat{k}_b)) + (C_1(K_i) - 2C_1(0))$$
$$\times D_\ell(K_f)P_\ell(\hat{K}_f.\hat{k}_b)\} - 4\pi\{C_2(q) - 2(C_2(K_i) + C_2(K_f))$$
$$+ C_1(K_f)C_2(K_i) + C_1(K_i)C_2(K_f)\}D_0(0)\Big], \quad (20)$$

where M_C corresponds to the contribution in the usual second Born amplitude f_{B2} which is evaluated by following the method of Ehrhardt *et al* [17] and Baliyan and Srivastava [18]. The second part in (20) represents the correction due to the choice $\phi^{(-)}_{\mathbf{k}_b}(\mathbf{r})$ rather than the standard Coulomb wave $\phi^{(-)}_{C,\mathbf{k}_b}(\mathbf{r})$ for the ejected electron. The maximum value of ℓ in the summations over ℓ in (13) and (20) has been obtained by comparing the results with $\ell_{max} = 0$, 1 and 2. It is found that taking $\ell_{max} = 1$ is good enough for ejected electron energies E_b up to 10 eV. For larger E_b, a higher ℓ_{max} is perhaps needed. We have, however, taken $\ell_{max} = 2$ in all the cases considered here. The integration over $\mathbf{q}$ in (17) is performed numerically following Srivastava and Sharma [19].

3. Results

Figures 1–3 show our results in the coplanar geometry plotted against the ejected electron angle θ_b for (i) $\theta_a = 0{\cdot}35°$, $E_b = 5$ eV, (ii) $\theta_a = 0{\cdot}32°$, $E_b = 10$ eV and (iii) $\theta_a = 1°$, $E_b = 75$ eV respectively in the first Born approximation B1 (× × ×), second Born approximation B2 (○ ○ ○), improved first Born approximation CB1 (– – –) and improved second Born approximation CB2 (———). The scattered electron energy E_a in every case is 5·5 keV. The theoretical results have been normalized to the absolute experimental data of Dupre *et al* [11] for excitation to $n = 2$(s, p) by multiplying them by the factors shown in the figures. The recoil peak intensity naturally decreases in all cases as E_b increases. The second Born approximation leads to a decrease (increase) in

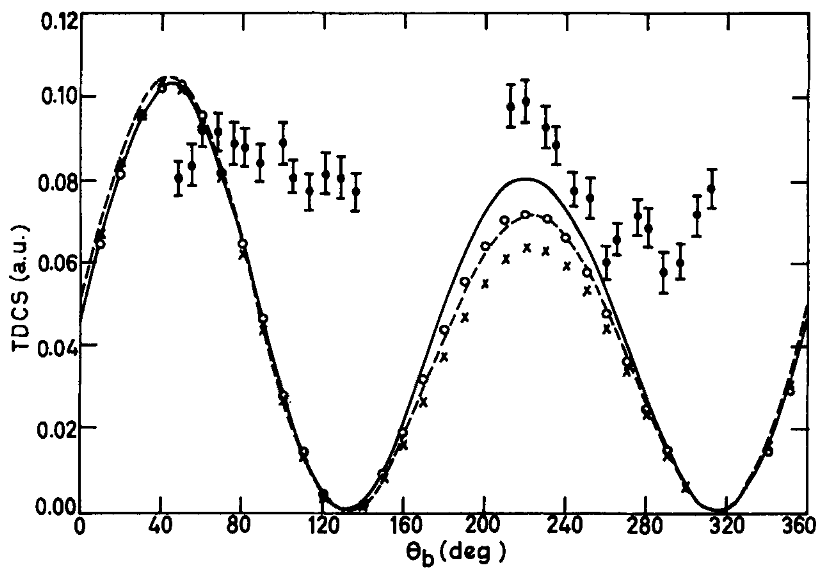

Figure 1. Triple differential cross sections (in a.u.) for the simultaneous ionization and excitation of helium by electron impact at $E_0 = 5570{\cdot}4$ eV, $E_b = 5$ eV and $\theta_a = 0{\cdot}35°$ plotted as a function of ejection angle θ_b. Theoretical results: × × × ×: (B1 × 0·182); – – – –: (CB1 × 0·238); ○ ○ ○ ○: (B2 × 0·190) and ———: (CB2 × 0·25). Experimental data are the absolute measurements of Dupre *et al* [11] for excitation to He^+(2s, 2p).

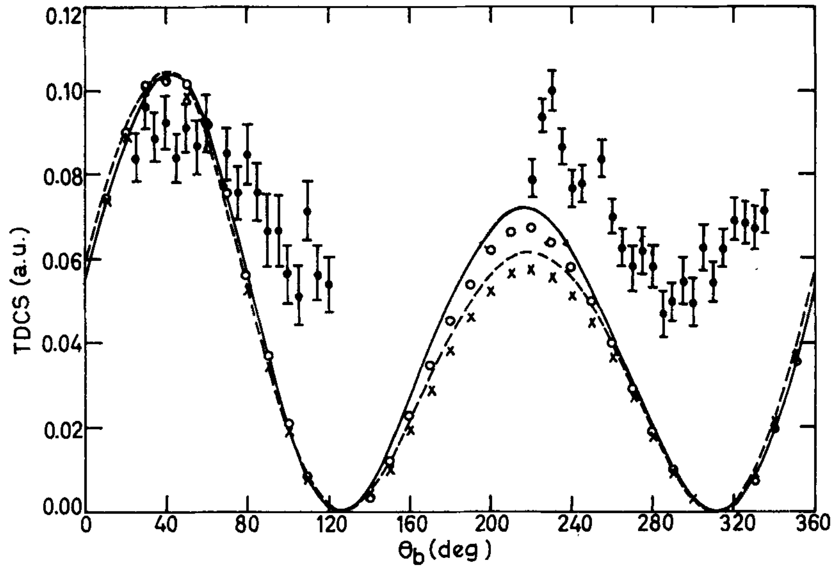

Figure 2. Same as figure 1 but for $E_0 = 5575{\cdot}4\,\text{eV}$, $E_b = 10\,\text{eV}$ and $\theta_a = 0{\cdot}32°$. Theoretical results: ××××: (B1 × 0·263); ----: (CB1 × 0·370); ○○○○: (B2 × 0·278) and ———: (CB2 × 0·40).

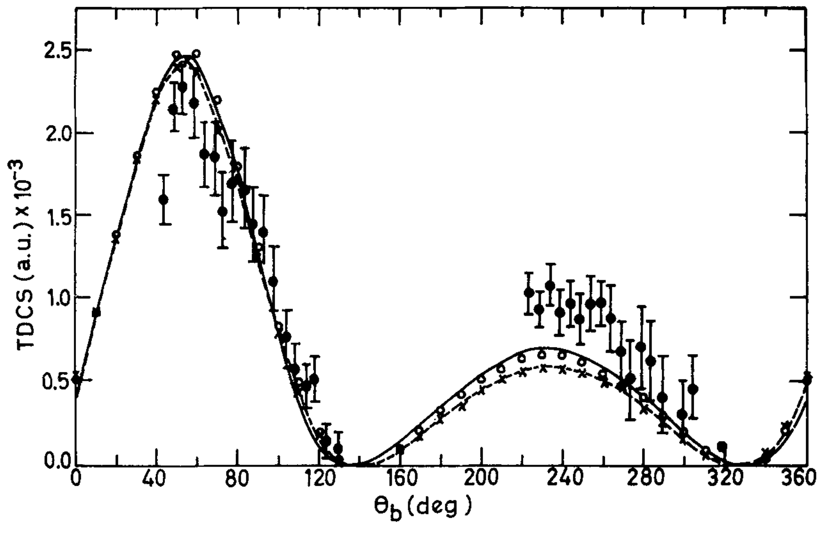

Figure 3. Same as figure 1 but for $E_0 = 5640{\cdot}4\,\text{eV}$, $E_b = 75\,\text{eV}$ and $\theta_a = 1°$. Theoretical results: ×××× : (B1 × 0·65); ----: (CB1 × 1·1); ○○○○: (B2 × 0·7) and ———: (CB2 × 1·2).

the binary (recoil) peak height. This feature is similar to what is found in the case of ionization without excitation. The ratio of the recoil peak to binary peak intensity increases by about 15% in B2 results over B1 at $E_b = 5\,\text{eV}$ (figure 1). This improvement is little less at $E_b = 10$ eV and $E_b = 75$ eV. The model CB2 leads to an improvement of about 30% in this ratio over the B1 results at $E_b = 5$ and 10 eV. At $E_b = 75$ eV (figure 3), the increase is less, about 12%. The experiments indicate a still larger recoil peak intensity. A possible reason for this inadequacy of the present model could be the use of average excitation energy $\bar{\omega}$ and closure used in the evaluation of the second Born term. A variation of $\bar{\omega}$ within the present model does not lead to much change in the results.

4. Conclusions

The 'improved' second Born approximation is found to increase the ratio of recoil peak to binary peak intensity quite a bit over the value obtained by using the first Born approximation. However this enhancement is not large enough to reproduce the experimental value. The present model also fails to reproduce shallow maxima and minima observed in the angular distribution of TDCS for small ejected electron energies. The second order term is thus important but not enough to reproduce the observed angular distribution of the cross section.

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