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Abstract

Recently, Lahmam-Bennani *et al* (2010 *J. Phys. B: At. Mol. Opt. Phys.* **43** 105201) have shown that the second Born approximation is necessary to describe the experimental results of the double ionization of atoms and molecules. The second Born approximation needs a difficult triple numerical integration and often many authors find some controversial results. We now investigate in a greater detail the application of the second Born approximation for the easier case: the ionization of atomic hydrogen by electrons. The ionization of atomic hydrogen allows us to check accurately this approximation because the wave functions describing the target are known exactly. Moreover**,** sophisticated models such as CCC and CDW-EIS exist and give closer results leading to easier comparisons. We report accurate second Born results for differential cross sections for the ionization of atomic hydrogen using a basis including 100 discrete states, and another basis including 32 discrete states and pseudo-states. The results of the present method are compared with other calculations and experiment. The single ionization of helium is also investigated in order to answer to an old controversy between two different theoretical results. Finally an application of the second Born approximation to the double ionization of helium has been performed.

PACS:34.80.Dp Keywords: single ionization, double ionization, second Born approximation.

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1. Introduction

The ionization of atoms and molecules by electrons or positrons is of great interest in astrophysics, plasma physics and radiation physics. The knowledge of single and double ionization is also needed in other sciences such as life science. Recent sophisticated theories such as exterior complex scaling (Rescigno *et al* 1999), time-dependent close coupling (Colgan and Pindzola 2006), convergent close coupling (Bray 2002), R matrix theory (Reid *et a*l 1998) are mostly successful in predicting cross sections for the ionization of hydrogen or helium but are not yet able to describe fully differential cross section for the double ionization of helium (Durr *et al* 2007, Pindzola *et al* 2008). Moreover**,** these theories can be applied, up to now and only for numerical reasons, to light atoms and to the simplest molecule H_2. In the other cases it is necessary to apply perturbation theories like the Born series.

Ionization of the atomic hydrogen by fast projectiles is a good check for a perturbation theory because experimental results exist, particularly for the triple differential cross sections (Weigold *et al* 1979, Lohmann *et al* 1984, Ehrhardt *et al* 1985, Ehrhardt *et al* 1986). In such an experiment the ejected electron is detected in coincidence with the scattered electron and it is well known (Ehrhardt *et al* 1986) that this kind of experiment, called (e, 2e) experiments, is very sensitive to the details of the theory. It is due to the fact that in the case of triple differential cross section, the theory is *directly* comparable to the experiments without averaging over unobserved parameters (unlike for the double or single differential cross sections, for instance). Weigold *et al* (1979) performed the first (e,2e) experiment on atomic hydrogen at incident energies of 100, 113.6, 250 and 413.6 eV while the energy of the ejected electron varied from 25 eV to 200 eV. Lohmann *et al* (1984) used more asymmetric conditions (250 eV for the incoming and 5, 10 and 14 eV respectively, for the ejected electron). Finally Ehrhardt *et al* (1985) reported the first *absolute* triple differential cross sections for asymmetric geometries (250 eV for the incident electron and 5 eV for the ejected electron). In all these experiments the kinematics is coplanar.

Byron *et al* (1980) were the first to apply the second Born approximation for the ionization of atomic hydrogen. Pathak and Srivastava (1981) used the second Born approximation for the ionization of the atomic hydrogen and compared their results to the first (e,2e) experiments of Weigold *et al* (1979) (at the incident energy of 250 eV and ejected electrons of 50 eV). Then they also made calculations for the ionization of helium by using the closure approximation and compared their results to those of Ehrhardt *et al* (1982). Byron *et al* (1982) also calculated triple differential cross sections for the ionization of helium by using the closure approximation and found results which disagreed with those of Pathak and Srivastava. Later on**,** Byron *et al* (1985) applied the second Born approximation by using very few discrete states as intermediate states and by taking into account the closure approximation and adding the contribution of the third Born approximation calculated with the Glauber approximation. It is time now to answer to several questions about the second Born approximation. The first is the number of discrete states which are necessary to be included in the calculation of the second Born approximation. A second question is the role played by the continuum states. We also must see what happens when we add pseudo-states as intermediate states.

In the present investigation we have performed a calculation by using the second Born approximation which includes 100 *exact* discrete states corresponding to n=1 to n=10. Then we also perform another calculation which uses both exact and pseudo-states. Finally we shall compare our results to those given by the 3C model (or BBK model) (Brauner *et al* 1989) which is considered as of infinite order when treating the interaction between the two outgoing electrons but in an approximate way.

We have also applied the second Born approximation to the double ionization of helium and compared our results to those of Lahmam-Bennani *et al* (2010) and Lahmam-Bennani *et al* (2002).

Atomic units are used throughout unless otherwise stated.

2. Theory

We first consider the ionization of atomic hydrogen by electrons

$$e^- + H \rightarrow 2\,e^- + H^+, \qquad (1)$$

In the second Born approximation, the triple differential cross section (TDCS) is given by

$$\sigma^{(3)} = \frac{d^3\sigma}{d\Omega_e d\Omega_s dE_e} = \frac{k_s k_e}{k_i} \left| f_{B1} + f_{B2} \right|^2, \qquad (2)$$

where $d\Omega_s$ and $d\Omega_e$ denote, respectively, the elements of solid angles for the scattered and the ejected electron whereas the energy interval of the ejected electron is represented by dE_e. The momenta of the incident, scattered, and ejected electrons are denoted by $\vec{k}_i$, $\vec{k}_s$ and $\vec{k}_e$, respectively.

The first Born term f_{B1} is given by

$$f_{B1} = -\frac{1}{2\pi}\left\langle \exp(i\vec{k}_s.\vec{r}_0)\Psi_C^-(\vec{k}_e,\vec{r}_1)\right| V \left| \exp(i\vec{k}_i.\vec{r}_0)\Phi_i(\vec{r}_1)\right\rangle, \qquad (3)$$

where $\Phi_i(\vec{r}_1)$ is the *exact* wave function of the initial state of the atomic hydrogen and $\Psi_C^-(\vec{k}_e,\vec{r}_1)$ is also the *exact* wave function for the continuum state of the atomic hydrogen given by

$$\Psi_C^-(\vec{k}_e,\vec{r}_1) = \frac{1}{(2\pi)^{3/2}}\exp(i\vec{k}_e.\vec{r}_1)\Gamma(1-i\alpha)\exp(-\frac{\pi}{2}\alpha)\,{}_1F_1\,(i\alpha,1,-i(\vec{k}_e.\vec{r}_1 + k_e r_1)), \quad \text{with} \quad \alpha = -Z/k_e,$$

and $Z = 1$.

The potential V represents the coulomb interaction between the incoming electron and the target and is written as

$$V = \frac{1}{r_{01}} - \frac{1}{r_0} \qquad (4)$$

We neglect the exchange effects by considering the scattered electron as the fast electron and the ejected electron as the slow electron. We can easily perform the integration over $\vec{r}_0$ analytically and get

$$f_{B1} = -\frac{2}{K^2}\left\langle \Psi_C^-(\vec{k}_e,\vec{r}_1)\middle| \exp(i\vec{K}.\vec{r}_1) - 1 \middle| \Phi_i(\vec{r}_1)\right\rangle , \quad (5)$$

where $\vec{K} = \vec{k}_i - \vec{k}_s$ is the momentum transfer.

Following Joachain (1983) the second Born term f_{B2} is given by

$$\begin{aligned} f_{B2} &= \frac{1}{8\pi^4}\sum_n \int \frac{d\vec{q}}{q^2 - k_n^2 - i\varepsilon} \\ &\left\langle \exp(i\vec{k}_s.\vec{r}_0)\Psi_C^-(\vec{k}_e,\vec{r}_1)\middle| V \middle| \exp(i\vec{q}.\vec{r}_0)\Phi_n(\vec{r}_1)\right\rangle , \\ &\left\langle \exp(i\vec{q}.\vec{r}_0)\Phi_n(\vec{r}_1)\middle| V \middle| \exp(i\vec{k}_i.\vec{r}_0)\Phi_i(\vec{r}_1)\right\rangle \end{aligned} \quad (6)$$

with $\varepsilon \to 0^+$ and

$$\frac{k_n^2}{2} = \frac{k_i^2}{2} - (E_n - E_i) \quad (7)$$

if we only consider the contributions of the n *exact* discrete states of the atomic hydrogen (n varying from n=1 to n$\to\infty$), E_n being the eigenvalue of the atomic hydrogen Hamiltonian corresponding to the eigenfunction Φ_n.

We also perform the integration over $\vec{r}_0$ and get

$$\begin{aligned} f_{B2} &= \frac{2}{\pi^2}\sum_n \int \frac{d\vec{q}}{q^2 - k_n^2 - i\varepsilon}\frac{1}{K_i^2 K_f^2} \\ &\left\langle \Psi_C^-(\vec{k}_e,\vec{r}_1)\middle| \exp(i\vec{K}_f.\vec{r}_1) - 1 \middle| \Phi_n(\vec{r}_1)\right\rangle \\ &\left\langle \Phi_n(\vec{r}_1)\middle| \exp(i\vec{K}_i.\vec{r}_1) - 1 \middle| \Phi_i(\vec{r}_1)\right\rangle \end{aligned} \quad (8)$$

where $\vec{K}_i = \vec{k}_i - \vec{q}$ and $\vec{K}_f = \vec{q} - \vec{k}_s$, $\vec{K} = \vec{K}_i + \vec{K}_f$. When we consider n different from n=1 we have the orthogonality of the initial state and other states (final or intermediate) and the term -1 (corresponding to the interaction of the electron with the target nucleus) present in (5) and (8) does not contribute.

When the contribution of the final continuum state is considered in the second Born term we must add the following term (Byron *et al* 1983)

$$f_{B2}^{C} = \frac{1}{8\pi^4}\int d\vec{p}\int \frac{d\vec{q}}{q^2 - \overline{k}^2 - i\varepsilon}$$
$$\left\langle \exp(i\vec{k}_s.\vec{r}_0)\Psi_C^-(\vec{k}_e,\vec{r}_1)\right| V \left|\exp(i\vec{q}.\vec{r}_0)\Psi_C^-(\vec{p},\vec{r}_1)\right\rangle \tag{9}$$
$$\left\langle \exp(i\vec{q}.\vec{r}_0)\Psi_C^-(\vec{p},\vec{r}_1)\right| V \left|\exp(i\vec{k}_i.\vec{r}_0)\Phi_i(\vec{r}_1)\right\rangle$$

with $\varepsilon \to 0^+$ and

$$\frac{\overline{k}^2}{2} = \frac{k_i^2}{2} - \frac{p^2}{2} - \frac{1}{2} \tag{10}$$

As pointed out by Byron *et al* (1983) the calculation of the off-shell free-free matrix element is a difficult task. Two ways are now possible to avoid the direct calculation of f_{B2}^{C}: the first is to consider the closure approximation and the second is to only use (8) but with pseudo-states.

The closure approximation consists in replacing the target energy difference $E_n - E_i$ by an average excitation energy $\overline{w}$ and summing over *all* the intermediate states $\sum_n \int |\Phi_n\rangle\langle\Phi_n| = 1$.

Consequently we get

$$\overline{f}_{B2} = \frac{2}{\pi^2}\int \frac{d\vec{q}}{q^2 - p^2 - i\varepsilon}\frac{1}{K_i^2 K_f^2}$$
$$\left\langle \Psi_C^-(\vec{k}_e,\vec{r}_1)\right| \exp(i\vec{K}_f.\vec{r}_1) - 1 \Big| \exp(i\vec{K}_i.\vec{r}_1) - 1 \left|\Phi_i(\vec{r}_1)\right\rangle \tag{11}$$

with $\varepsilon \to 0^+$ and

$$\frac{p^2}{2} = \frac{k_i^2}{2} - \overline{w} \tag{12}$$

We can rewrite (11) as

$$\overline{f}_{B2} = \frac{2}{\pi^2}\int \frac{d\vec{q}}{q^2 - p^2 - i\varepsilon}\frac{1}{K_i^2 K_f^2}$$
$$\left\langle \Psi_C^-(\vec{k}_e,\vec{r}_1)\right| \exp(i\vec{K}.\vec{r}_1) - \exp(i\vec{K}_f.\vec{r}_1) - \exp(i\vec{K}_i.\vec{r}_1) + 1 \left|\Phi_i(\vec{r}_1)\right\rangle \tag{13}$$

Byron and Joachain (1966) have also proposed another formulation of the closure approximation: they exactly include some contributions from the low-lying discrete states (generally n=1 and n=2). To perform this task they have to calculate

$$\bar{f}_{B2}^{BJ} = \bar{f}_{B2} - f_{B2}^{n=1}(\overline{w}) + f_{B2}^{n=1} - f_{B2}^{n=2}(\overline{w}) + f_{B2}^{n=2} + ... \tag{14}$$

In (14) $f_{B2}^{n=1}(\overline{w})$ corresponds to (8) with n=1 (it is an elastic collisions as a first collision) with

$$\frac{k_{n=1}^2}{2} = \frac{k_i^2}{2} - (\overline{w}) \tag{15}$$

The term $f_{B2}^{n=2}(\overline{w})$ means

$f_{B2}^{n=2}(\overline{w}) = f_{B2}^{2s}(\overline{w}) + f_{B2}^{2p_0}(\overline{w}) + f_{B2}^{2p_1}(\overline{w}) + f_{B2}^{2p_{-1}}(\overline{w})$, as for $f_{B2}^{n=2}$.

Secondly we consider the single ionization of the helium atom by electrons

$$e^- + He \rightarrow 2\, e^- + He^+, \tag{16}$$

for which the final state of the ion He^+ is in its ground state (1s).

The first Born term f_{B1} is now given by

$$f_{B1} = -\frac{1}{2\pi}\left\langle \exp(i\vec{k}_s.\vec{r}_0)\Psi_f(\vec{r}_1,\vec{r}_2)\right| V \left| \exp(i\vec{k}_i.\vec{r}_0)\Phi_i(\vec{r}_1,\vec{r}_2)\right\rangle, \tag{17}$$

where $\Phi_i(\vec{r}_1,\vec{r}_2)$ is the wave function of the initial state of the helium atom and $\Psi_f(\vec{r}_1,\vec{r}_2)$ is the wave function of the final target system consisting of a He^+ (1s) ion and an unbound electron. The potential V represents the Coulomb interaction between the incoming electron and the target and is written as

$$V = \frac{1}{r_{01}} + \frac{1}{r_{02}} - \frac{2}{r_0} \tag{18}$$

For the initial state we use an analytical fit to the Hartree-Fock wave function (Byron and Joachain 1966)

$\Phi_i(\vec{r}_1,\vec{r}_2) = \phi_0(\vec{r}_1)\phi_0(\vec{r}_2)$ where $\phi_0(\vec{r}\,) = (4\pi)^{-1/2}(A\exp(-\alpha r) + B\exp(-\beta r))$

with $A = 2.60505$, $B = 2.08144$, $\alpha = 1.41$ and $\beta = 2.61$.

The final state wave function is a symmetrised product of the He^+ ground-state wave function for the bound electron multiplied by a Coulomb wave function orthogonalized to the helium ground state as in Byron *et al* (1986)

$$\Psi_f(\vec{r}_1,\vec{r}_2)=\frac{1}{\sqrt{2}}\left[\Psi_C^{-\perp}(\vec{k}_e,\vec{r}_1)\phi_n(\vec{r}_2)+\Psi_C^{-\perp}(\vec{k}_e,\vec{r}_2)\phi_n(\vec{r}_1)\right]$$

with $\left|\Psi_C^{-\perp}\right\rangle=\left|\Psi_C^{-}\right\rangle-\left\langle\phi_0\middle|\Psi_C^{-}\right\rangle\left|\phi_0\right\rangle$.

Performing the integration on $\vec{r}_0$ in equation (17) one can write the first Born term as

$$\begin{aligned} f_{B1} = -\frac{2^{3/2}}{K^2}\Big[& \left\langle\Psi_C^{-}(\vec{k}_e)\right|\exp(i\vec{K}.\vec{r})\left|\phi_0\right\rangle \\ & -\left\langle\Psi_C^{-}(\vec{k}_e)\middle|\phi_0\right\rangle\left\langle\phi_0\right|\exp(i\vec{K}.\vec{r}\left|\phi_0\right\rangle\Big]\left\langle\phi_n\middle|\phi_0\right\rangle \end{aligned}, \tag{19}$$

Following Joachain (1983) the second Born term f_{B2} is given by

$$\begin{aligned} f_{B2} = & \frac{1}{8\pi^4}\sum_n\int\frac{d\vec{q}}{q^2-k_n^2-i\varepsilon} \\ & \left\langle\exp(i\vec{k}_s.\vec{r}_0)\Psi_f(\vec{r}_1,\vec{r}_2)\right|V\left|\exp(i\vec{q}.\vec{r}_0)\Phi_n(\vec{r}_1,\vec{r}_2)\right\rangle, \\ & \left\langle\exp(i\vec{q}.\vec{r}_0)\Phi_n(\vec{r}_1,\vec{r}_2)\right|V\left|\exp(i\vec{k}_i.\vec{r}_0)\Phi_i(\vec{r}_1,\vec{r}_2)\right\rangle \end{aligned} \tag{20}$$

with $\varepsilon\to 0^+$ and

$$\frac{k_n^2}{2}=\frac{k_i^2}{2}-(E_n-E_i) \tag{21}$$

where E_n is the eigenvalue of the helium atom Hamiltonian corresponding to the eigenfunction Φ_n.

Performing the integration over $\vec{r}_0$ in equation (20) one can write the second Born term as

$$\begin{aligned} f_{B2} = & \frac{2}{\pi^2}\sum_n\int\frac{d\vec{q}}{q^2-k_n^2-i\varepsilon}\frac{1}{K_i^2K_f^2} \\ & \left\langle\Psi_f(\vec{r}_1,\vec{r}_2)\right|\exp(i\vec{K}_f.\vec{r}_1)+\exp(i\vec{K}_f.\vec{r}_2)-2\left|\Phi_n(\vec{r}_1,\vec{r}_2)\right\rangle, \\ & \left\langle\Phi_n(\vec{r}_1,\vec{r}_2)\right|\exp(i\vec{K}_i.\vec{r}_1)+\exp(i\vec{K}_i.\vec{r}_2)-2\left|\Phi_i(\vec{r}_1,\vec{r}_2)\right\rangle \end{aligned} \tag{22}$$

Now, by applying the closure approximation we get

$$\begin{aligned} \bar{f}_{B2} = & \frac{2}{\pi^2}\int\frac{d\vec{q}}{q^2-p^2-i\varepsilon}\frac{1}{K_i^2K_f^2} \\ & \left\langle\Psi_f(\vec{r}_1,\vec{r}_2)\right|\exp(i\vec{K}_f.\vec{r}_1)+\exp(i\vec{K}_f.\vec{r}_2)-2\Big| \\ & \Big|\exp(i\vec{K}_i.\vec{r}_1)+\exp(i\vec{K}_i.\vec{r}_2)-2\left|\Phi_i(\vec{r}_1,\vec{r}_2)\right\rangle \end{aligned} \tag{23}$$

with $\varepsilon\to 0^+$ and

$$\frac{p^2}{2} = \frac{k_i^2}{2} - \overline{w} \tag{24}$$

$\overline{w}$ being the average excitation energy. After some straightforward algebra the expression (23) can be reduced to

$$\begin{aligned}
\bar{f}_{B2} = \frac{2^{3/2}}{\pi^2} \int \frac{d\vec{q}}{q^2 - p^2 - i\varepsilon} \frac{1}{K_i^2 K_f^2} \\
[\langle \Psi_C^- | \exp(i\vec{K}.\vec{r}) | \phi_0 \rangle \langle \phi_n | \phi_0 \rangle + \langle \Psi_C^- | \exp(i\vec{K}_f.\vec{r}) | \phi_0 \rangle \langle \phi_n | \exp(i\vec{K}_i.\vec{r}) | \phi_0 \rangle + \\
\langle \Psi_C^- | \exp(i\vec{K}_i.\vec{r}) | \phi_0 \rangle \langle \phi_n | \exp(i\vec{K}_f.\vec{r}) | \phi_0 \rangle - 2 \langle \Psi_C^- | \exp(i\vec{K}_f.\vec{r}) | \phi_0 \rangle \langle \phi_n | \phi_0 \rangle \\
- 2 \langle \Psi_C^- | \exp(i\vec{K}_i.\vec{r}) | \phi_0 \rangle \langle \phi_n | \phi_0 \rangle - \langle \Psi_C^- | \phi_0 \rangle \langle \phi_0 | \exp(i\vec{K}.\vec{r}) | \phi_0 \rangle \langle \phi_n | \phi_0 \rangle \\
+ 2 \langle \Psi_C^- | \phi_0 \rangle \langle \phi_0 | \exp(i\vec{K}_i.\vec{r}) | \phi_0 \rangle \langle \phi_n | \phi_0 \rangle \\
+ 2 \langle \Psi_C^- | \phi_0 \rangle \langle \phi_0 | \exp(i\vec{K}_f.\vec{r}) | \phi_0 \rangle \langle \phi_n | \phi_0 \rangle \\
- \langle \Psi_C^- | \phi_0 \rangle \langle \phi_0 | \exp(i\vec{K}_i.\vec{r}) | \phi_0 \rangle \langle \phi_n | \exp(i\vec{K}_f.\vec{r}) | \phi_0 \rangle \\
- \langle \Psi_C^- | \phi_0 \rangle \langle \phi_0 | \exp(i\vec{K}_f.\vec{r}) | \phi_0 \rangle \langle \phi_n | \exp(i\vec{K}_i.\vec{r}) | \phi_0 \rangle]
\end{aligned} \tag{25}$$

This last expression is simpler than that found by Byron *et al* (1986).

Finally we consider the double ionization of helium by electrons

$$e^- + He \rightarrow 3\ e^- + He^{++}. \tag{26}$$

In the second Born approximation the fivefold differential cross section (FDCS) is given by

$$\sigma^{(5)} = \frac{d^5\sigma}{d\Omega_a d\Omega_b d\Omega_s dE_a dE_b} = \frac{k_s k_a k_b}{k_i} | f_{B1} + f_{B2} |^2, \tag{27}$$

where $d\Omega_s, d\Omega_a$ and $d\Omega_b$ denote, respectively, the elements of solid angles for the scattered and the ejected electrons a and b whereas the energy intervals of the ejected electrons are represented by dE_a and dE_b. The momenta of the incident, scattered, and ejected electrons are denoted by $\vec{k}_i$, $\vec{k}_s$, $\vec{k}_a$ and $\vec{k}_b$, respectively.

The first Born term f_{B1} is given here by

$$f_{B1} = -\frac{1}{2\pi} \langle \exp(i\vec{k}_s.\vec{r}_0) \Psi_f^{\perp}(\vec{k}_a, \vec{r}_1, \vec{k}_b, \vec{r}_2) | V | \exp(i\vec{k}_i.\vec{r}_0) \Phi_i(\vec{r}_1, \vec{r}_2) \rangle, \tag{28}$$

where $\Phi_i(\vec{r}_1,\vec{r}_2)$ is the wave function of the initial state of the helium atom and $\Psi_f^{\perp}(\vec{k}_a,\vec{r}_1,\vec{k}_b,\vec{r}_2)$ is the wave function for the double continuum state of the helium atom which is orthogonalized to the initial state. The potential *V* represents the coulomb interaction between the incoming electron and the target and is given by (18).

For the initial state we use an accurate Hylleraas-type wave function given by Bonham and Kohl (1966)

$$\Phi_i(\vec{r}_1,\vec{r}_2) = N_0\left[\exp(-ar_1-br_2)+\exp(-ar_2-br_1)+\beta\exp(-\gamma r_{12})\exp(-\alpha(r_1+r_2)\right] = \Phi_i^{BK14}$$

N_0 being a normalization factor and r_{12} the electron-electron distance, $a=1.3991$, $b=2.097$, $\alpha=1.63$, $\beta=-0.4431$ and $\gamma=0.4134$. The energy of the initial state given by this wave function is E=-2.903115 au. We also use a wave function which only includes a part of the radial correlation

$$\Phi_i(\vec{r}_1,\vec{r}_2) = N_0^{'}\left[\exp(-a^{'}r_1-b^{'}r_2)+\exp(-a^{'}r_2-b^{'}r_1)\right] = \Phi_i^{BK7}$$

where $a^{'}=1.1885$, $b^{'}=2.1832$ and which is often used actually (Ciappina *et al* 2008). The energy of the initial state given by this wave function is E=-2.875661 au.

The final state wave function is the approximate BBK wave function (Dal Cappello *et al* 1993) such that $\left|\Psi_f^{\perp}\right\rangle = \left|\Psi_f\right\rangle - \left\langle\Phi_i\middle|\Psi_f\right\rangle\left|\Phi_i\right\rangle$

$$\Psi_f(\vec{k}_a,\vec{r}_1,\vec{k}_b,\vec{r}_2) = \frac{1}{\sqrt{2}}\left[\Psi_C^-(\vec{k}_a,\vec{r}_1)\Psi_C^-(\vec{k}_b,\vec{r}_2)+\Psi_C^-(\vec{k}_a,\vec{r}_2)\Psi_C^-(\vec{k}_b,\vec{r}_1)\right]\varphi(\left|\vec{k}_a-\vec{k}_b\right|)$$

where $\varphi(\left|\vec{k}_a-\vec{k}_b\right|)$ is the repulsive Gamow factor $\varphi(\left|\vec{k}_a-\vec{k}_b\right|) = \exp(-\frac{\pi\chi_{ab}}{2})\Gamma(1-i\chi_{ab})$ and

$$\chi_{ab} = \frac{1}{\left|\vec{k}_a-\vec{k}_b\right|}.$$

If we neglect the exchange effects by considering the scattered electron as the fast electron and the ejected electrons as the slow electrons we can easily perform the integration over $\vec{r}_0$ analytically and get

$$f_{B1} = -\frac{2}{K^2}\left\langle\Psi_f^{\perp}(\vec{k}_a,\vec{r}_1,\vec{k}_b,\vec{r}_2)\middle|\exp(i\vec{K}.\vec{r}_1)+\exp(i\vec{K}.\vec{r}_2)-2\middle|\Phi_i\right\rangle, \qquad (29)$$

The second Born term f_{B2} is given by

$$f_{B2} = \frac{1}{8\pi^4} \sum_n \int \frac{d\vec{q}}{q^2 - k_n^2 - i\varepsilon}$$
$$\left\langle \exp(i\vec{k}_s.\vec{r}_0)\Psi_f^{\perp}(\vec{k}_a,\vec{r}_1,\vec{k}_b,\vec{r}_2)\right| V \left|\exp(i\vec{q}.\vec{r}_0)\Phi_n(\vec{r}_1,\vec{r}_2)\right\rangle \tag{30}$$
$$\left\langle \exp(i\vec{q}.\vec{r}_0)\Phi_n(\vec{r}_1,\vec{r}_2)\right| V \left|\exp(i\vec{k}_i.\vec{r}_0)\Phi_i(\vec{r}_1,\vec{r}_2)\right\rangle$$

where the summation over n means that we take into account all the contributions of the n discrete and continuum states of the helium atom. It means that the incident electron collides twice with the target and corresponds to the well-known two-step 2 mechanism (TS2) (Carlson and Krause 1965). Performing the integration on $\vec{r}_0$ in equation (30) and applying the closure approximation we get (Grin *et al* 2000)

$$\bar{f}_{B2} = \frac{2}{\pi^2} \int \frac{d\vec{q}}{q^2 - p^2 - i\varepsilon} \frac{1}{K_i^2 K_f^2}$$
$$\left\langle \Psi_f^{\perp}(\vec{k}_a,\vec{r}_1,\vec{k}_b,\vec{r}_2)\right| \exp(i\vec{K}_f.\vec{r}_1) + \exp(i\vec{K}_f.\vec{r}_2) - 2 \Big| \tag{31}$$
$$\Big| \exp(i\vec{K}_i.\vec{r}_1) + \exp(i\vec{K}_i.\vec{r}_2) - 2 \left|\Phi_i(\vec{r}_1,\vec{r}_2)\right\rangle$$

and

$$\frac{p^2}{2} = \frac{k_i^2}{2} - \overline{w} \tag{32}$$

$\overline{w}$ being the average excitation energy.

It is important to note that all integrals on $d\vec{q}$ must be performed numerically with great care (see appendix).

3. Results and discussion

a) Ionization of atomic hydrogen by electrons

We investigate the ionization of atomic hydrogen by electrons by comparing the results of our second Born approximation with the absolute data of Ehrhardt *et al* (1985, 1986). The incident energy is 250 eV and the ejected electron has an energy of 5 eV. First, we consider the case where the incoming electron is scattered at $\theta_s = 3^0$ which corresponds to a low momentum transfer

(K=0.27 au). Next**,** we need to know if it is necessary to include many discrete states as intermediate states in the second Born approximation. In figure 1a we compare the results of the first Born treatment with those of the second Born by including successively n=1, n=2 and n=3 as intermediate states. It is clear that the contribution of the elastic case (n=1) plays no important role here. We only notice a small rise of the amplitude of the recoil peak. When we add the contribution of the excited states corresponding to n=2 (2s and 2p) we observe a fall of the binary lobe amplitude and a rise of the recoil lobe amplitude. As a matter of fact the most important contribution is due to the 2p excited state (see table 1). This result is easy to understand because it corresponds to the dipolar transition $1s \rightarrow 2p$ which is important for low momentum transfer. This result was also noticed by Byron *et al* (1985). Now if we add the contribution of the excited states corresponding to n=3 we clearly see that the increasing of the recoil lobe amplitude continues as the decreasing of the binary peak amplitude. It is true that the contribution of n=2 is the most important but not sufficient, and that the contribution from n=3 must be added.

Figure 1b shows the contributions of the excited states corresponding to n=4 and n=5. We only see a small contribution from these excited states. Clearly**,** the n=5 excited state gives no contribution for the binary peak and shows a very small decreasing of the recoil peak amplitude. It seems that we have reached the convergence limit of the contribution of the discrete states. In order to check this point we draw in figure 1c the contributions of n=6**,** n=7, n=8, n=9, and n=10 (which correspond to 100 discrete states). It is conspicuous that the contributions from n=7 to n=10 play no significant role here and can be neglected (see table 2).

If we consider another case where the momentum transfer is bigger (for example $\theta_s = 8^0$ which corresponds to a momentum transfer K=0.61 au) we find the same results as before and conclude that the convergence is reached by adding contributions up to n=6.

Now we investigate the closure approximation with the same kinematical conditions. Figure 2 shows the results of the closure approximation. We observe that the closure approximation using equation (13) or equation (14) gives close results. In our case equation (14) is calculated with n=1 to n=6 (Byron *et al* (1985) only include n=1 and n=2). From this figure it appears that the results given by the closure approximation are different from those given by the contributions of the discrete states (from n=1 to n=6). It means that we cannot neglect the contributions of the continuum states. It was also the conclusion of Byron *et al* (1985). It was written in the paper of Byron *et al* (1985) that their results of their second Born calculation were insensitive to the variation of $\overline{w}$. We find that it is not the case with our calculations: figure 3 shows that the change of the value of the parameter changes the values of the results of our second Born calculation. We also perform, like Byron *et al* (1985), calculations with $\overline{w}$ =0.5 au and $\overline{w}$ =1 au but by including more discrete states. We can conclude from the results of the closure approximation that the contributions due to the continuum states are necessary and that, unhappily the closure approximation depends on the choice of the parameter $\overline{w}$. This result was also found by Lahmam-Benanni *et al* (2003) for the double ionization of helium by electrons. Another way to include these contributions from the continuum states is to consider a basis with pseudo-states. Hence we consider two pseudo-states basis which include 31 (Callaway 1978) and 32 (Callaway 1993) states, respectively. The eigenvalues vary from -0.5 au to 1.02 au (Callaway 1978) and from -0.5 au to 4.8 au (Callaway 1993). Further details of these two basis can be found in Rouet (1996).

Figure 4 shows the results of the second Born approximation calculated with pseudo-states basis. We see that the contributions due to the continuum states are important for the binary peak as well for the recoil peak. A basis which only includes *discrete* excited states and pseudo-states is never able to fully reproduce the decrease of the binary peak and the increase of the recoil peak. The two basis of Callaway (1978 and 1993) including positive eigenvalues give close results particularly for the binary peak.

From the results of the closure approximation and those of the pseudo-states basis it is now clear that the continuum states play a role in the ionization of the atomic hydrogen for these particular kinematical conditions (large incident energy compared to the energy of the ejected electron).

It is now time to compare our theoretical results to the well-known BBK model (Brauner *et al* 1989) and to the absolute data of Ehrhardt (1985, 1986). We have followed the recommendation of Jones and Madison (2002) and multiplied all the data by a scaling factor of 0.88. Jones and Madison (2000) find a very good agreement between their CDW-EIS model (Crothers and Mc Cann 1983, Jones and Madison 1998), which contains the same BBK wave function for the final state with an eikonal initial state instead of the plane wave for the incident electron, with the nonperturbative Convergent Close Coupling model (CCC) (Bray *et al* 1994, Jones and Madison 2000). From this good agreement between the two theories (CDW-EIS and CCC) they conclude that the experimental data of Ehrhardt *et al* (1985, 1986) must be multiplied by a scaling factor of 0.88. For the incident energy considered here (250 eV) the BBK model and CDW-EIS yield results which are in close agreement with those of the most sophisticated Convergent Close Coupling model (CCC) (Jones and Madison 2000). Figure 5 shows such a comparison for $\theta_s = 3^0$. The agreement is very good between the results of the BBK model, those of the second Born approximation with the closure approximation and the experiments. As seen above the second Born approximation calculated only with the discrete states (n=1 to n=6, or n=1 to n=10) is insufficient: the contribution of the continuum states is necessary. This contribution is included in the BBK model because the interaction between the scattered electron and the ejected electron is treated to an infinite order but in an approximate way.

Figure 6 shows a comparison between our second Born treatment with pseudo-states, the BBK model and experiments ($\theta_s = 3^0$). We notice a very good agreement between the BBK model, our second Born approximation with pseudo-states and experiments. Here the contributions of the continuum states are important, particularly for the binary peak.

Figures 7 and 8 show the results of the second Born approximation and the BBK model for the ionization of the hydrogen atom for an incident energy of 250 eV and an ejected energy of 50 eV. The relative experiments of Weigold *et al* (1979) have been normalized to the BBK model at $\theta_s = 25^0$ and $\theta_e = 60^0$. These experiments are interesting because Pathak and Srivastava (1981) conclude that the second Born approximation is not able to bring about a general improvement in the values of the TDCS over the first Born results. These authors use the closure approximation with a high average excitation energy $\overline{w}$ =1 au**.** It was the start of a controversy with Byron *et al* (1982) who claimed that the closure approximation can only be justified if the energy of the ejected electron is small (and the scattering angle is small too). Figure 7a shows our results of the second Born approximation with the contributions of the n=1, n=2 and n=3 intermediate states for $\theta_s = 15^0$. Once again we notice that the contribution of n=1 is very small but, in this case, the other contributions (n=2 and n=3) are small too. Figure 7b shows that the second Born approximation calculated by including only the contributions of discrete states (n=1 to n=6) is insufficient to describe the experiments. The closure approximation (calculated with $\overline{w}$ =0.5 au) completely fails as claimed by Byron *et al* (1982). The shift of the binary peak is not reproduced contrary to the BBK model which predicts a significant shift. In figure 7c we see that the second Born approximation calculated by including discrete states and pseudo-states brings no improvement. We also notice that the exchange effects are small here (BBK model with exchange) and can be neglected. Figure 8a for $\theta_s = 25^0$ confirms that the closure approximation fails. The second Born approximation calculated by including only the contributions of discrete states (n=1 to n=6) gives a magnitude which is less than those given by the first Born approximation (contrary to the closure approximation). In figure 8b we notice that the second Born approximation calculated by including discrete states and pseudo-states overestimate the experiments. Finally the BBK model or the BBK model with exchange give the best agreement with experiments (the exchange effects are small too). Pathak and Srivastava (1981) and Byron *et al* (1982) were right: the second Born approximation is not working when the energy of the ejected electrons is not small. If the BBK model gives a good agreement it means that we need to take into account higher order of the interaction between the scattered electron and the ejected electron.

b) Ionization of atomic hydrogen by positrons

The ionization of atomic hydrogen by positrons is a more difficult problem because rearrangement collisions are possible due to positronium formation. Hence the ionization of atomic hydrogen by positrons is a two-center collision system while the ionization of atomic hydrogen is a single-center one. Although much progress has been made (see for instance Kadyrov *et al* 2007) we observe that the problem of the ionization of atomic hydrogen by positrons is not yet solved. Brauner *et al* (1989) have applied their BBK model to the ionization of atomic hydrogen by positrons and obtain the TDCS. Bandyopadhyay *et al* (1994) and Fiol and Olson (2002) also used the BBK model for the calculations of the triple differential cross sections and double differential cross sections. But, up to now, none has applied the second Born approximation for the ionization of atomic hydrogen by positrons (Sharma and Srivastava (1988) have applied the second Born approximation for the ionization of *helium* by electrons and positrons). In our Born approximation plane waves are used for the incident and scattered particles. It may be noted that the first Born amplitude term has opposite signs for positron and electron impacts. If we only consider the first Born approximation we find the same cross section for electron impact or positron impact because the triple differential cross section is directly connected to the square of the first Born term (see equation (2)). The sign of the second Born term does not depend on the charge of the particle but now the sign of the first Born term plays a role because the first Born term is added to the second Born term, explaining the change of behaviour when the second Born approximation is applied for electron impact and positron impacts.

Figure 9 shows the results of our BBK model (which yields the same values as those found by Brauner *et al* (1989)) along with our second Born treatment. For $\theta_s = 3^0$ we observe the same trends: the second Born approximation with the closure approximation or with the pseudo-states gives a good agreement with the BBK model and our second Born treatment, which only includes the contributions of the eigenstates n=1 to n=6, underestimates the binary peak. Generally speaking the second Born approximation gives an enhanced binary peak and a reduced recoil peak in contrast to the results of the first Born approximation. It is exactly the inverse result for electron impact.

c) Single ionization of helium by electrons

We now investigate the single ionization of helium by electrons by comparing the results of our second Born approximation with the relative data of Ehrhardt *et al* (1982) and a first theoretical calculation of Pathak and Srivastava (1981) using the closure approximation with $\overline{w}$ =1.3 au and a second theoretical calculation of Byron *et al* (1982) using the same closure approximation but with $\overline{w}$ =0.9 au. These two groups use the same theoretical expression (25). Figure 10 shows the results of the first and second Born approximation with the two values of the parameter $\overline{w}$. We only notice small differences between the two calculations and find results close to those of Byron *et al* (1982): the first and second Born triple differential cross sections differ by only 17% at the binary peak, with the second Born result being smaller than the first Born result (as in the case of atomic hydrogen).We also find that the ratio of the binary peak to the recoil peak is reduced from the first Born value of 8.43 to the second Born value of 5.63 in better agreement with experiment. Thus, as written by Byron *et al* (1982), the results of Pathak and Srivastava (1981) in this case are *incorrect*. The results of the BBK model are also drawn in Figure 10. Binary to recoil peak ratio of 4.21 given by the BBK model is approaching the experimental value. Once again we can conclude that the contributions of the continuum states are necessary because these contributions are assumed in the BBK model.

Figure 11 shows that all the terms of equation (3) in appendix contribute to the second Born approximation: if we neglect, for instance (like Fang and Bartschat 2001), the most difficult term (the triple numerical integral, equation (4) in appendix) we see practically no shift for the recoil lobe. We find that the maximum of the recoil lobe is located at $\theta_e = 105^0$ (first born approximation), $\theta_e = 110^0$ (second born approximation without the triple numerical integral) while the second Born approximation and the BBK model gives the maximum close to $\theta_e = 130^0$. As a matter of fact the large shift of the recoil peak is generally due to the triple numerical integral in equation (4) and can never be deleted.

d) Double ionization of helium by electrons and positrons

We finally investigate the double ionization of helium by electrons (or by positrons) by comparing the results of our second Born approximation with the relative data of Lahmam-Bennani *et al* (2002) and Lahmam-Bennani *et al* (2010). In these experiments the slow ejected electron is not detected and we must integrate the equation (27) over the solid angle $d\Omega_b$. The large angular shifts of the forward and backward lobes with respect to the momentum transfer direction were questioned by Götz *et al* (2003). Figure 12 shows that the second Born approximation is now able to reproduce the shift of the binary peak and describe partially the shift of the recoil peak. We also see that the results of the second Born approximation depend on the choice of the wave function used: the BK14 wave function reproduces a minimum around 310^0 as the experiments, contrary to the BK7 wave function which exhibits a maximum. But no model has yet been able to reproduce *all* the data. Furthermore, we notice that even the most sophisticated model DS6C of Götz *et al* (2006) fails to describe the strong violation of the first Born symmetry seen in the experiment. The relative good agreement between our model and the experiment means that the TS2 mechanism (which is implicitly included in the second Born approximation) plays an important role here. Figure 13 shows the results of our second Born approximation (by using the closure approximation) with the latest results of Lahmam-Bennani *et al* (2010). We notice a good agreement, particularly for the large angular shift of the binary peak. We also study the double ionization of helium by positrons. In this case the amplitude of the binary peak increases while the amplitude of the recoil peak decreases. This is exactly what we observe when we investigate the single ionization of atomic hydrogen by electrons and positrons. In figure 14 we study the role played by the average excitation energy $\overline{w}$. As for the case of the ionization of atomic hydrogen we find that the results depend on this value: we notice a change of the shape for $\overline{w}$ =30 eV. In this case the maximum at 210^0

disappears and becomes a minimum. These results confirm those found by Lahmam-Benanni *et al* (2003). It means that it is here important to include the contributions of all states before using the closure approximation but it is a difficult problem, particularly when we want to take into account of the single and double continuum states and the resonances.

4. Conclusion

The second Born approximation has been first studied for the ionization of atomic hydrogen using a large number of intermediate states. The results show that the contributions from the discrete states are insufficient and the continuum states must be added. We confirm the first results of Byron, Joachain and Piraux: the contribution of the n=2 as an intermediate state is the most important one. Nevertheless**,** it is necessary to add the n=3, n=4, n=5 and n=6 contributions and those of the continuum states. The closure approximation, which is often used (Marchalant *et al* 1999, Marchalant *et al* 2000, Kheifets 2004, Grin *et al* 2000, Choubisa *et al* 2003), works very well for small energy of the ejected electrons. For higher ejection energies this approximation completely fails. The second Born approximation using discrete states in conjunction with pseudo-states gives better agreement in some cases but is not always sufficient to describe experiments. This result proves again that the contributions of the continuum states must be added and it is certainly necessary to consider more and more pseudo-states. The second Born approximation works for the ionization of targets by positrons as the BBK model. Although the BBK model gives here a good agreement with experiments it was noticed by Dey *et al* (2008) that the recent experiments of the ionization of helium by electrons (Catoire *et al* 2006, Stevenson *et al* 2007) are not well described by this model which overestimates the differential cross sections in the recoil region. Moreover Dal Cappello *et al* (2008) show that the ionization-excitation of helium cannot be described by the BBK model, contrary to a model using the second Born approximation (Watanabe *et al* 2007). The second Born approximation works quite well for the double ionization of helium by using the closure approximation with particular values of the average excitation energy $\overline{w}$. The big shift of the binary peak found experimentally by Lahmam-Bennani *et al* (2010) is well reproduced showing that the TS2 mechanism is very important in this case.

Acknowledgments

We would like to thank B Piraux and Yu V Popov for helpful discussions. We also thank the PMMS (Pôle Messin de Modélisation et de Simulation) for computer time.

Appendix

As pointed out by Byron *et al* (1985) *great care* must be taken while carrying out the integration on $d\vec{q}$ since *the integrand is singular* at $q = p$ (equations (11), (13), (23), and (25)) or $q = k_n$ (equations (6), (8), (20), and (22)) or $q = \bar{k}$ (equation (9)) and *is also singular* at $\vec{q} = \vec{k}_i$ and $\vec{q} = \vec{k}_s$. The last two singularities are not difficult for numerical integration. Interestingly, as written by Marchalant *et al* (1998), these singularities are only apparent and can be overcome by using prolate spheroidal coordinates. We can also use the well-known integration formulas of Gaussian type to avoid these two particular singularities. The first singularity is more difficult for numerical integration. As proposed by Piraux (1983) the general integral

$$I = \int \frac{d\vec{q}}{q^2 - p^2 - i\varepsilon} W(q, \theta_q, \varphi_q) \quad (1)$$

with $\varepsilon \to 0^+$ can be performed by using

$$\frac{1}{q^2 - p^2 - i\varepsilon} = P\left(\frac{1}{q^2 - p^2}\right) + i\pi\delta(q^2 - p^2) \quad (2)$$

where P stands for the principal value. Then we rewrite I as

$$I = P\int \frac{d\vec{q}}{q^2 - p^2} W(q,\theta_q,\varphi_q) + \frac{i\pi}{2} p \int d\hat{q}\, W(p,\theta_q,\varphi_q) \qquad (3)$$

The second term is easy to calculate contrary to the principal value which is sometimes neglected (Fang and Bartschat 2001) or approximated by using a peaking approximation (Franz and Altick 1995).

Following Piraux (1983) the principal part is written as

$$J = P\int \frac{q^2 dq}{q^2 - p^2} \int_{-1}^{+1} G(q,\cos(\theta_q))\, d(\cos(\theta_q)) \qquad (4)$$

and

$$G(q,\cos(\theta_q)) = \int_0^{2\pi} W(q,\theta_q,\varphi_q)\, d\varphi_q \qquad (5)$$

Finally, after some algebra (Piraux 1983)

$$J = \left(\int_0^{p-\varepsilon'} + \int_{p+\varepsilon'}^{\infty} \right) \frac{q^2 dq}{q^2 - p^2} \int_{-1}^{+1} G(q,\cos(\theta_q))\, d(\cos(\theta_q)) + \left(\frac{\varepsilon' J_0}{2p} + \varepsilon' J_1 \right) \qquad (6)$$

with

$$J_0 = \int_{-1}^{+1} H(p,\cos(\theta_q))\, d(\cos(\theta_q)) , \qquad (7)$$

$$J_1 = \int_{-1}^{+1} d(\cos(\theta_q)) \frac{\partial}{\partial q} H(q,\cos(\theta_q))_{q=p} \qquad (8)$$

and

$$H(q,\cos(\theta_q)) = qG(q,\cos(\theta_q)) \qquad (9)$$

Marchalant *et al* (1998) adopt a subtraction procedure to evaluate (3) and introduce an exponential factor to make the integrals convergent as $q \to \infty$:

$$I = \left(P\int_0^{\infty} \frac{\exp(-\alpha(q-p)^2)q^2 dq}{q^2-p^2} + \frac{i\pi p}{2} \right) \int W(p,\theta_q,\varphi_q)d\hat{q}$$
$$+ \int \frac{(W(q,\theta_q,\varphi_q) - \exp(-\alpha(q-p)^2)W(p,\theta_q,\varphi_q))}{q^2-p^2} d\vec{q} \tag{10}$$

The parameter α in (10) is free of choice and the results should be independent of it (Marchalant *et al* 1998).

As a check on the accuracy of our numerical procedures we have calculated the most singular integral contained in the above expressions following Byron *et al* (1985)

$$I_0 = \int \frac{d\vec{q}}{q^2 - p^2 - i\varepsilon} \frac{1}{K_i^2 K_f^2}, \tag{11}$$

with $\varepsilon \to 0^+$.

This integral can be exactly evaluated by using the results of Lewis (1956)

if $k_s \langle p \langle k_i$, then

$$I_0 = \frac{i\pi^2}{K\sqrt{\Delta}} Ln\left[\frac{(pK + \sqrt{\Delta})^2}{\left|k_i^2 - p^2\right|\left|p^2 - k_s^2\right|} \right], \tag{12}$$

where $\Delta = K^2 p^2 + (p^2 - k_i^2)(p^2 - k_s^2)$.

If $p \langle k_s$, then

$$I_0 = \frac{i\pi^2}{K\sqrt{\Delta}} Ln\left[\frac{(pK + \sqrt{\Delta})^2}{\left|k_i^2 - p^2\right|\left|p^2 - k_s^2\right|} \right] + \frac{\pi^3}{K\sqrt{\Delta}}, \tag{13}$$

If $p = k_s$, then the imaginary part of I_0 tends to infinity and the real part is

$$R_e(I_0) = \frac{\pi^3}{2pK^2}, \tag{14}$$

And if $p = k_i$, the imaginary part of I_0 tends to the infinity and the real part is

$$R_e(I_0) = -\frac{\pi^3}{2pK^2}, \tag{15}$$

Generally we have to deal with the expression (12) and we get an accuracy of 10^{-5} by using typically 500000 quadrature points for the triple numerical integration.

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Figure captions

Figure 1a: Triple differential cross section (TDCS) for ionization of atomic hydrogen by 250 eV electron impact for $\theta_s = 3^0$ as a function of the ejected electron angle θ_e relative to the incident electron direction. The ejected electron energy is $E_e = 5$ eV. The results of the first Born approximation are represented by a full curve, those of the second Born approximation calculated by including only the contribution of the target ground state (n=1) by a dashed line, those of the second Born approximation calculated by including only the contributions n=1 and n=2 by a dotted line and those of the second Born approximation calculated by including only the contributions n=1, n=2 and n=3 by a dash-dotted line.

Figure 1b: Same as figure 1a but the results of the second Born approximation calculated by including only the contribution of n=1, n=2 and n=3 are represented by a dashed line, those of the second Born approximation calculated by including only the contributions n=1, n=2 , n=3 and n=4 by a dotted line and those of the second Born approximation calculated by including only the contributions n=1, n=2 , n=3 , n=4 and n=5 by a dash-dotted line.

Figure 1c: Same as figure 1a but the results of the second Born approximation calculated by including only the contributions of n=1, n=2 and n=3 are represented by a dashed line, those of the second Born approximation calculated by including only the contributions n=1, n=2, n=3 , n=4, n=5 and n=6 by a dotted line and those of the second Born approximation calculated by including all the contributions from n=1 to n=10 by a dash-dotted line.

Figure 2: Triple differential cross section (TDCS) for ionization of atomic hydrogen by 250 eV electron impact for $\theta_s = 3^0$ as a function of the ejected electron angle θ_e relative to the incident electron direction. The ejected electron energy is $E_e = 5$ eV. The results of the first Born approximation are represented by a full curve, those of the second Born approximation calculated by including only the contributions n=1, n=2, n=3, n=4, n=5 and n=6 by a dashed line, those of the second Born approximation calculated by using the closure approximation (equation (13)) by a

dotted line and those of the second Born approximation calculated by using the closure approximation (equation (14)) by a dash-dotted line.

Figure 3: Triple differential cross section (TDCS) for ionization of atomic hydrogen by 250 eV electron impact for $\theta_s = 3^0$ as a function of the ejected electron angle θ_e relative to the incident electron direction**.** The ejected electron energy is $E_e = 5$ eV. The results of the first Born approximation are represented by a full curve, those of the second Born approximation calculated by including only the contributions n=1, n=2, n=3, n=4, n=5 and n=6 by a dashed line, those of the second Born approximation calculated by using the closure approximation (equation (13), $\overline{w} = 0.5\,\text{au}$) by a dotted line and those of the second Born approximation calculated by using the closure approximation (equation (13), $\overline{w} = 1\,\text{au}$) by a dash-dotted line.

Figure 4: Triple differential cross section (TDCS) for ionization of atomic hydrogen by 250 eV electron impact for $\theta_s = 3^0$ as a function of the ejected electron angle θ_e relative to the incident electron direction. The ejected electron energy is $E_e = 5$ eV. The results of the first Born approximation are represented by a full curve, those of the second Born approximation calculated by including only *discrete* eigenstates and pseudo-states (Callaway 1978) by a dashed line and by a short-dashed line (Callaway 1993), those of the second Born approximation calculated by including all the eigenstates and pseudo-states (Callaway 1978) by a dotted line and by a short-dotted line (Callaway 1993).

Figure 5: Triple differential cross section (TDCS) for ionization of atomic hydrogen by 250 eV electron impact for $\theta_s = 3^0$ as a function of the ejected electron angle θ_e relative to the incident electron direction. The ejected electron energy is $E_e = 5$ eV. The results of the first Born approximation are represented by a full curve, those of the second Born approximation calculated by including only discrete states (n=1 to n=6) by a dashed line, those of the second Born approximation calculated by the closure approximation ($\overline{w} = 0.5\,\text{au}$) by a dotted line, those of the BBK model by a dash-dotted line and experiments (multiplied by 0.88) by squares.

Figure 6: Triple differential cross section (TDCS) for ionization of atomic hydrogen by 250 eV electron impact for θ_s =3^0 as a function of the ejected electron angle θ_e relative to the incident electron direction. The ejected electron energy is $E_e = 5$ eV. The results of the first Born approximation are represented by a full curve, those of the second Born approximation calculated by including only *discrete* eigenstates and pseudo-states (Callaway 1993) by a dashed line, those of the second Born approximation calculated by including all the eigenstates and pseudo-states (Callaway 1993) by a dotted line, those of the BBK model by a dash-dotted line and experiments (multiplied by 0.88) by squares.

Figure 7a: Triple differential cross section (TDCS) for ionization of atomic hydrogen by 250 eV electron impact for θ_s =15^0 as a function of the ejected electron angle θ_e relative to the incident electron direction. The ejected electron energy is $E_e = 50$ eV. The results of the first Born approximation are represented by a full curve, those of the second Born approximation calculated by including only the contribution of the target ground state (n=1) by a dashed line, those of the second Born approximation calculated by including only the contributions n=1 and n=2 by a dotted line and those of the second Born approximation calculated by including only the contributions n=1, n=2 and n=3 by a dash-dotted line.

Figure 7b: Triple differential cross section (TDCS) for ionization of atomic hydrogen by 250 eV electron impact for θ_s =15^0 as a function of the ejected electron angle θ_e relative to the incident electron direction. The ejected electron energy is $E_e = 50$ eV. The results of the first Born approximation are represented by a full curve, those of the second Born approximation calculated by including only the contribution of the discrete states (n=1 to n=6) by a dashed line, those of the second Born approximation calculated by using the closure approximation (equation (13)) by a dotted line, those of the second Born approximation calculated by using the closure approximation (equation (14)) by a dash-dotted line, those of the BBK model by a short dotted line and experiments (multiplied by 0.00224) by squares.

Figure 7c: Triple differential cross section (TDCS) for ionization of atomic hydrogen by 250 eV electron impact for $\theta_s = 15^0$ as a function of the ejected electron angle θ_e relative to the incident electron direction. The ejected electron energy is $E_e = 50$ eV. The results of the first Born approximation are represented by a full curve, those of the second Born approximation calculated by including only the contribution of the discrete states (n=1 to n=6) by a dashed line, those of the second Born approximation calculated by including all the eigenstates and pseudo-states (Callaway 1993) by a short dashed line, those of the BBK model by a dotted line and those by the BBK model with exchange by a dash-dotted line. Experiments (multiplied by 0.00224) are represented by squares.

Figure 8a: Same as figure 7b except for $\theta_s = 25^0$.

Figure 8b: Same as figure 7c except for $\theta_s = 25^0$.

Figure 9: Triple differential cross section (TDCS) for ionization of atomic hydrogen by 250 eV positron impact for $\theta_s = 3^0$ as a function of the ejected electron angle θ_e relative to the incident positron direction**.** The ejected electron energy is $E_e = 5$ eV. The results of the first Born approximation are represented by a full curve, those of the second Born approximation calculated by including only discrete states (n=1 to n=6) by a dashed line, those of the second Born approximation calculated by using the closure approximation by a dotted line, those of the second Born approximation calculated by including all the eigenstates and pseudo-states (Callaway 1993) by a short dashed line, and those of the BBK model by a dash-dotted line.

Figure 10: Triple differential cross section (TDCS) for the single ionization of helium by 500 eV electron impact for $\theta_s = 10.5^0$ as a function of the ejected electron angle θ_e relative to the incident electron direction. The ejected electron energy is $E_e = 5$ eV. The results of the first Born approximation are represented by a full curve, those of the second Born approximation calculated by using the closure approximation (equation (13)) with $\overline{w} = 0.9$ au) by a dashed line, those of the second Born approximation calculated by using the closure approximation (equation (13)) with

$\overline{w} = 1.3$ au by a dotted line and those of the BBK model by a dash-dotted line. Experiments (Ehrhardt *et al* 1982) are represented by squares and are normalised to the second Born approximation ($\overline{w} = 0.9$ au) at θ_e =280^0.

Figure 11: Triple differential cross section (TDCS) for ionization of helium by 500 eV electron impact for θ_s =10.5^0 as a function of the ejected electron angle θ_e relative to the incident electron direction**.** The ejected electron energy is $E_e = 5$ eV. The results of the first Born approximation are represented by a full curve, those of the second Born approximation calculated by using the closure approximation (equation (13)) with $\overline{w} = 1.3$ au) by a dashed line, those of the second Born approximation calculated by using the closure approximation without the triple numerical integral as (Fang and Bartschat 2001) (equation (13)) with $\overline{w} = 1.3$ au by a dotted line.

Figure 12: Fourfold differential cross section (4DCS) for the (e,3-1e) double ionization of helium by 640 eV electron impact for θ_s =1.5^0 and φ_s =180^0 as a function of the (fast) ejected electron angle θ_a relative to the incident electron direction. The fast ejected electron energy is $E_a = 51$ eV while the slow ejected electron energy is $E_b = 10$ eV. The results of the first Born approximation are represented by a full curve, those of the second Born approximation calculated by using the closure approximation (equation (31)) with $\overline{w} = 79$ eV and the BK14 initial wave function by a dotted line, those of the second Born approximation calculated by using the closure approximation (equation (31)) with $\overline{w} = 79$ eV and the BK7 initial wave function by a dashed line. The full squares are the experimental results of Lahmam-Bennani *et al* (2002).

Figure 13: Fourfold differential cross section (4DCS) for the (e, 3-1e) double ionization of helium by 621 eV electron and positron impact. Ejected electron energies are 37 eV and 5 eV. The scattering angle is θ_s =6^0 (φ_s =180^0). The 4DCS is plotted in polar coordinates as a function of the direction $\vec{k}_a$ of the fast ejected electron. The incident electron is moving along the x-axis. The x-axis and y-axis represent (4DCS) $\cos\theta_a$ and (4DCS) $\sin\theta_a$ respectively. The results of the first Born approximation are represented by a full curve, those of the second Born approximation for

electron impact and calculated by using the closure approximation (equation (31)) with $\overline{w} = 79\,\mathrm{eV}$ and the BK14 initial wave function by a dotted line, those of the second Born approximation for positron impact and calculated by using the closure approximation (equation (31)) with $\overline{w} = 79\,\mathrm{eV}$ and the BK14 initial wave function by a dashed line. The full squares are the experimental results of Lahmam-Bennani *et al* (2010).

Figure 14: Fourfold differential cross section (4DCS) for the (e, 3-1e) double ionization of helium by 621 eV electron impact. Ejected electron energies are 37 eV and 5 eV. The scattering angle is θ_s =6^0 (φ_s =180^0). The results of the first Born approximation are represented by a full curve, those of the second Born approximation calculated by using the closure approximation (equation (31)) with $\overline{w} = 79\,\mathrm{eV}$ and the BK14 initial wave function by a dashed line, those of the second Born approximation calculated by using the closure approximation (equation (31)) with $\overline{w} = 30\,\mathrm{eV}$ and the BK14 initial wave function by a dotted line, those of the second Born approximation calculated by using the closure approximation (equation (31)) with $\overline{w} = 116\,\mathrm{eV}$ and the BK14 initial wave function by a dash-dotted line.

Table 1

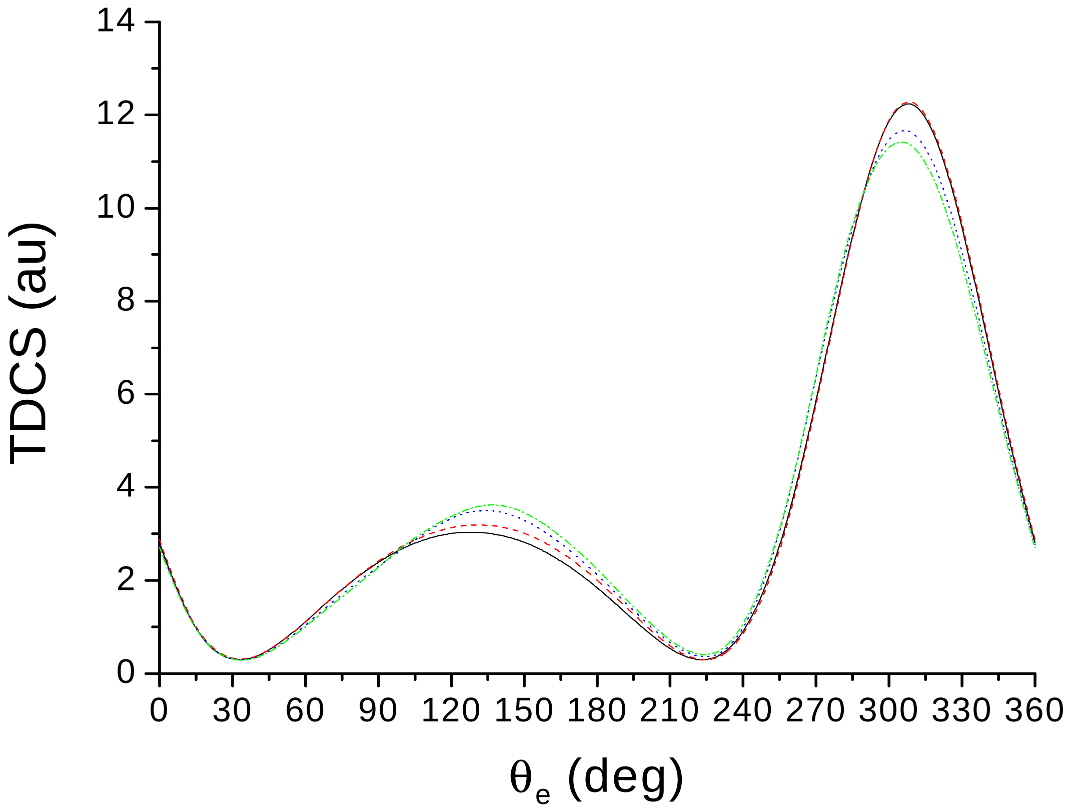
θ_e (deg)	B1	B2(1s)	B2(2s)	B2(2p)	SB2(0.5)	SB2(1.0)	B2(0.5)	B2(1.0)
10	1.363	1.409	1.323	1.362	0.597	0.974	0.599	1.019
30	0.247	0.261	0.235	0.250	0.296	0.443	0.289	0.433
50	0.666	0.660	0.670	0.620	0.808	0.885	0.790	0.897
70	1.581	1.576	1.573	1.495	1.577	1.695	1.552	1.758
90	2.400	2.427	2.340	2.334	2.489	2.578	2.446	2.619
110	2.906	2.996	2.834	3.037	3.467	3.354	3.401	3.129
130	3.050	3.210	2.985	3.418	4.248	3.895	4.281	3.701
150	2.830	3.026	2.712	3.229	4.456	4.010	4.618	4.225
170	2.253	2.438	2.106	2.556	3.830	2.438	4.030	2.106
190	1.387	1.521	1.270	1.589	2.455	2.355	2.605	2.758
210	0.510	0.567	0.458	0.630	0.932	1.010	1.000	1.207
230	0.313	0.286	0.314	0.370	0.446	0.442	0.489	0.538
250	1.885	1.800	1.932	2.100	2.265	1.876	2.369	1.978
270	5.823	5.747	5.995	6.272	6.139	5.502	6.113	5.077
290	10.54	10.53	10.64	10.44	9.302	9.185	9.183	8.982
310	12.41	12.46	12.39	11.74	9.058	9.811	9.034	10.19
330	9.675	9.756	9.600	9.129	5.934	6.948	5.948	7.376
350	4.847	4.922	4.779	4.665	2.504	3.234	2.511	3.445

Table 2

θ_e (deg)	B1	B2(2)	B2(3)	B2(4)	B2(5)	B2(6)	B2(8)	B2(10)
10	1.363	1.366	1.349	1.352	1.347	1.349	1.346	1.346
30	0.247	0.252	0.250	0.249	0.248	0.248	0.247	0.247
50	0.666	0.618	0.598	0.588	0.583	0.579	0.576	0.574
70	1.581	1.482	1.433	1.410	1.394	1.386	1.377	1.374
90	2.400	2.302	2.283	2.296	2.307	2.297	2.282	2.291
110	2.906	3.056	3.099	3.131	3.152	3.153	3.148	3.150
130	3.050	3.515	3.609	3.640	3.662	3.676	3.692	3.697
150	2.830	3.312	3.474	3.561	3.609	3.640	3.672	3.686
170	2.253	2.598	2.736	2.810	2.852	2.878	2.907	2.921
190	1.387	1.608	1.703	1.755	1.784	1.801	1.820	1.829
210	0.510	0.638	0.692	0.723	0.742	0.756	0.768	0.774
230	0.313	0.346	0.396	0.423	0.438	0.447	0.456	0.460
250	1.885	2.068	2.172	2.194	2.196	2.204	2.214	2.220
270	5.823	6.370	6.408	6.411	6.424	6.416	6.376	6.388
290	10.54	10.52	10.54	10.55	10.56	10.56	10.56	10.55
310	12.41	11.77	11.46	11.29	11.20	11.15	11.09	11.06
330	9.675	9.135	8.879	8.755	8.685	8.651	8.611	8.590
350	4.847	4.670	4.573	4.530	4.507	4.493	4.477	4.469

Table 1 Triple differential cross section (in au) for the ionization of atomic hydrogen as obtained from the second Born expressions (8), (13) and (14), using various approximations for $\bar{f}_{B2}$: SB2(0.5), $\bar{f}_{B2}$:calculated by the closure approximation using an average excitation energy $\overline{w} = 0.5$ au, SB2(1.0), $\bar{f}_{B2}$:calculated by the closure approximation using an average excitation energy $\overline{w} = 1.0$ au ; B2(1s), f_{B2} calculated by including only the contribution of the target ground state (1s) as an intermediate state; B2(2s) (B2(2p)), same calculation, in which only the contribution of the 2s(2p) state is included in f_{B2} ; B2(0.5), full second Born approximation results in which $\bar{f}_{B2}^{BJ}$ is calculated by including exactly the 1s, 2s and 2p intermediate target states, and the closure approximation (with $\overline{w} = 0.5$ au) is used to include the other target states; B2(1.0), full second Born approximation results in which $\bar{f}_{B2}^{BJ}$ is calculated by including exactly the 1s, 2s and 2p intermediate target states, and the closure approximation (with $\overline{w} = 1.0$ au) is used to include the other target states.B1: results of the first Born approximation (5). The incident electron energy is 250 eV, the ejected electron energy is 5 eV and the scattering angle $\theta_s = 3^0$.

Table 2 Triple differential cross section (in au) for the ionization of atomic hydrogen as obtained from the second Born expression (8), using various approximations for f_{B2} : B2(2) calculated by including only the contributions of n=1 and n=2; B2(3) calculated by including only the contributions of n=1, n=2 and n=3; B2(4) calculated by including only the contributions of n=1, n=2, n=3 and n=4; B2(5) calculated by including only the contributions of n=1, n=2, n=3, n=4 and n=5; B2(6) calculated by including only the contributions of n=1, n=2, n=3, n=4, n=5 and n=6; B2(8) calculated by including only the contributions of n=1, n=2, n=3, n=4, n=5, n=6, n=7 and n=8; B2(10) calculated by including only the contributions of n=1, n=2, n=3, n=4, n=5, n=6, n=7, n=8, n=9 and n=10. B1: results of the first Born approximation (5). The incident electron energy is 250 eV, the ejected electron energy is 5 eV and the scattering angle $\theta_s = 3^0$.



TDCS (au)
14
12
10
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6
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150
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210
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270
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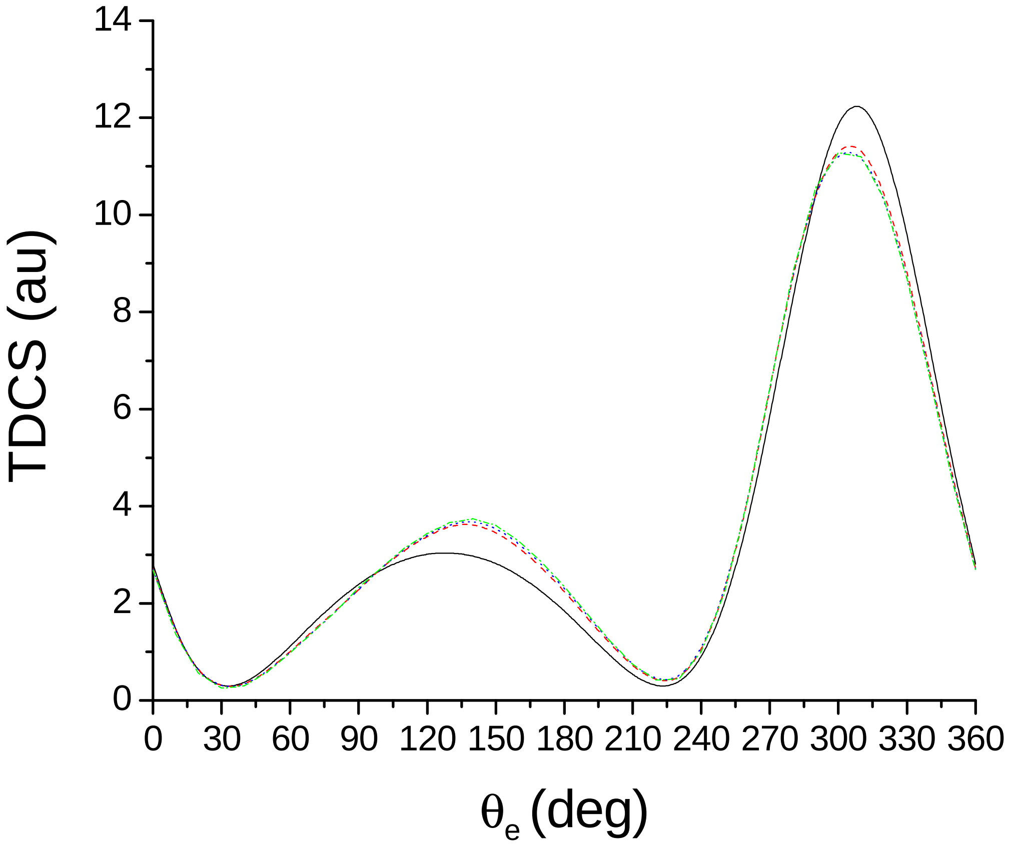
330
360
θe (deg)

Figure 1a



TDCS (au)
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2
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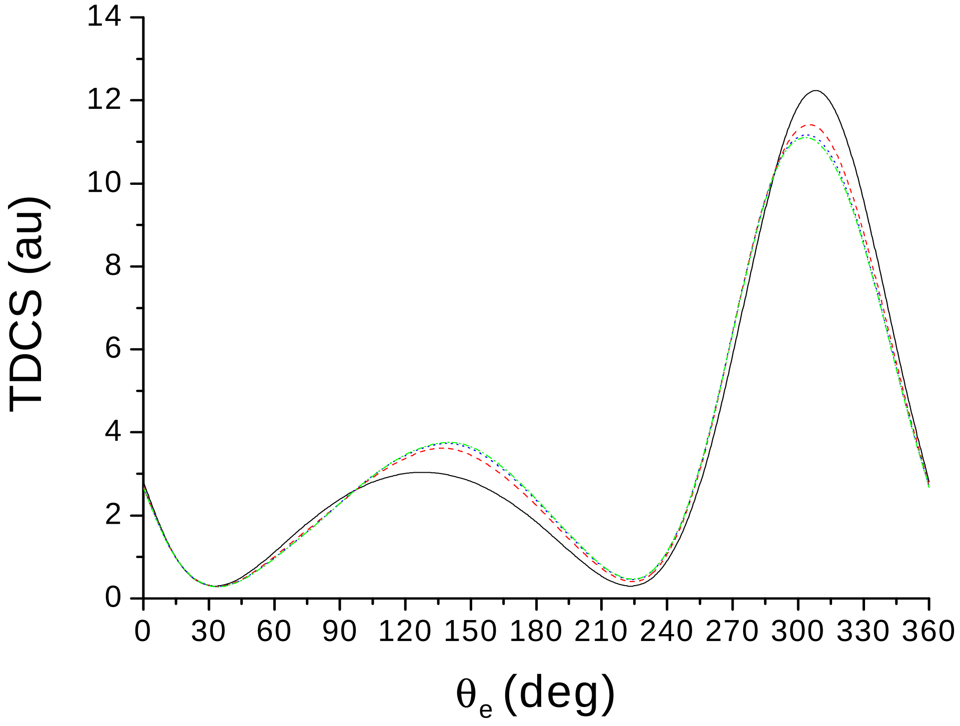
6
8
10
12
14
0 30 60 90 120 150 180 210 240 270 300 330 360
θe (deg)

Figure 1b



TDCS (au)
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2
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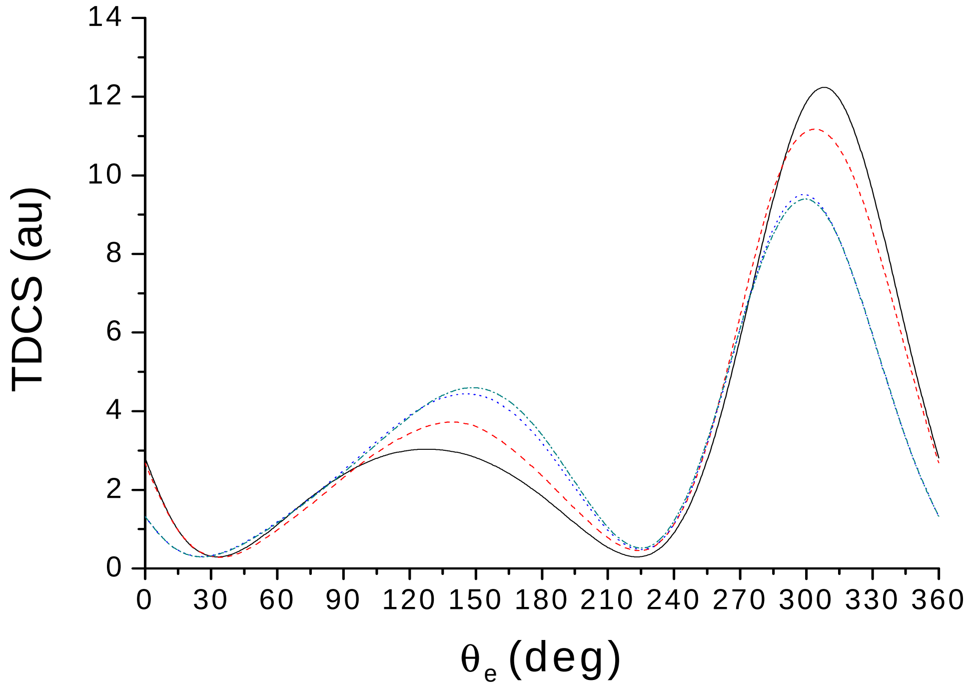
6
8
10
12
14
0 30 60 90 120 150 180 210 240 270 300 330 360
θe (deg)

Figure 1c



TDCS (au)
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150
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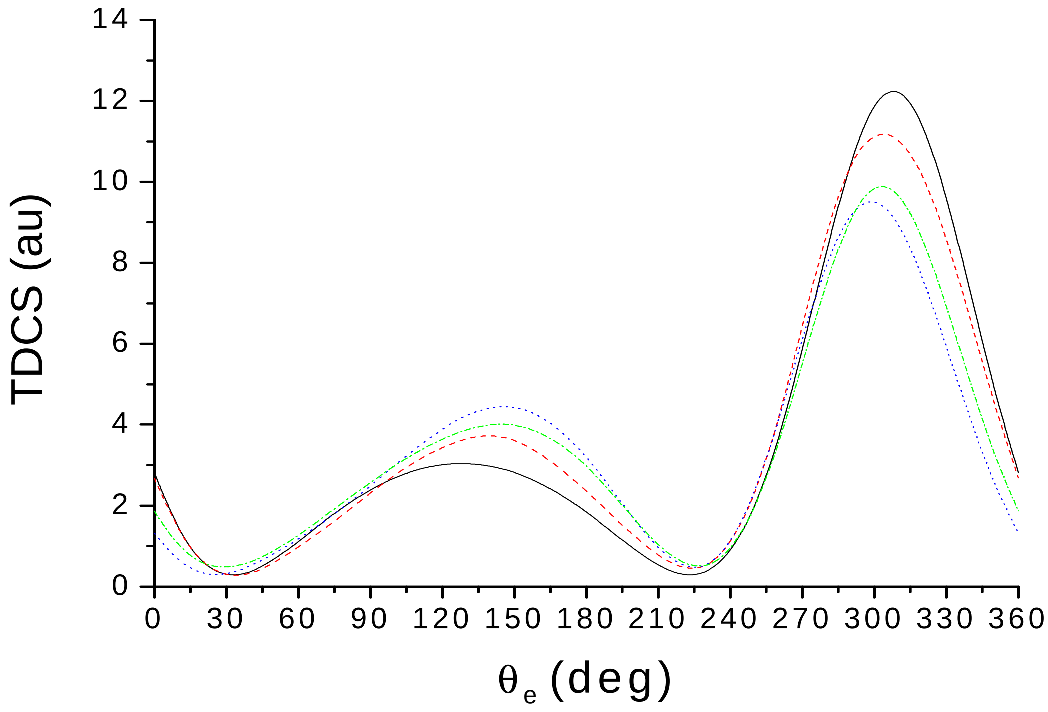
240
270
300
330
360
θ_e (deg)

Figure 2



TDCS (au)
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120
150
180
210
240
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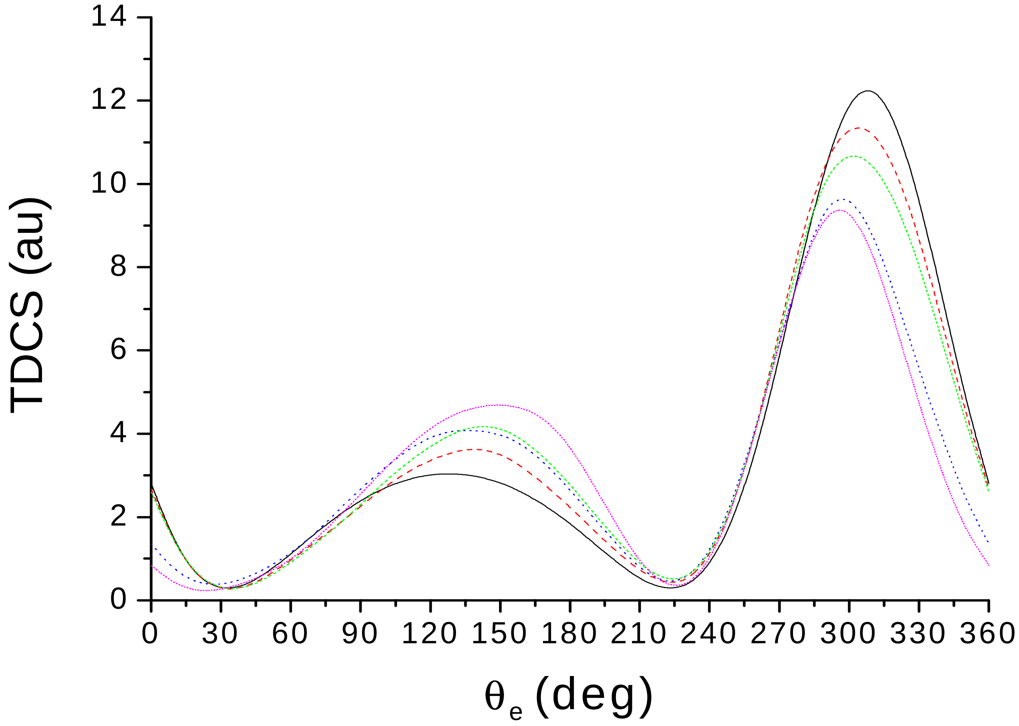
360
θ_e (deg)

Figure 3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12
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0
TDCS (au)
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90
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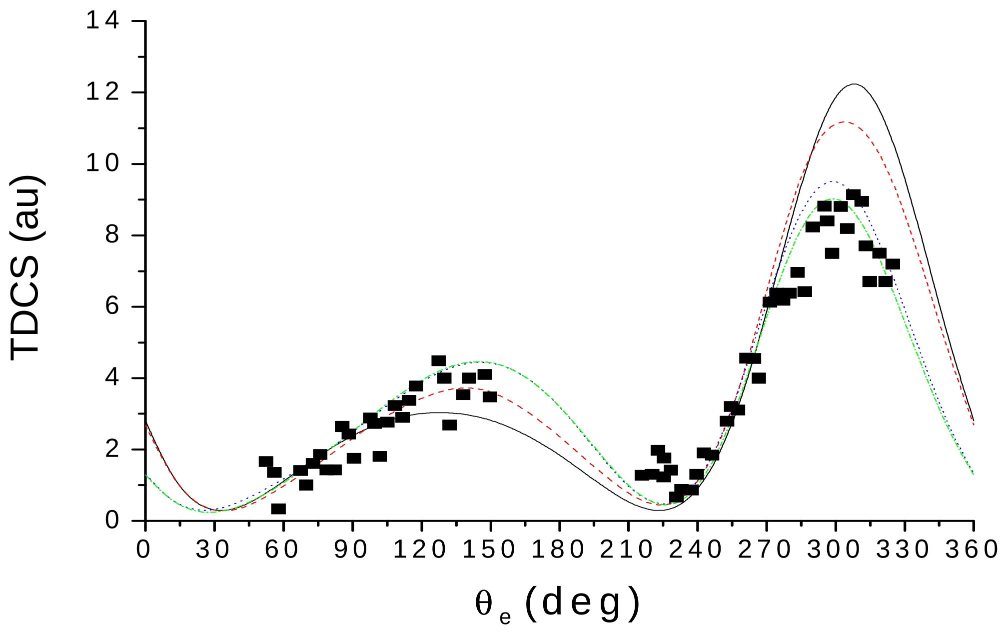
330
360
θe (deg)

Figure 4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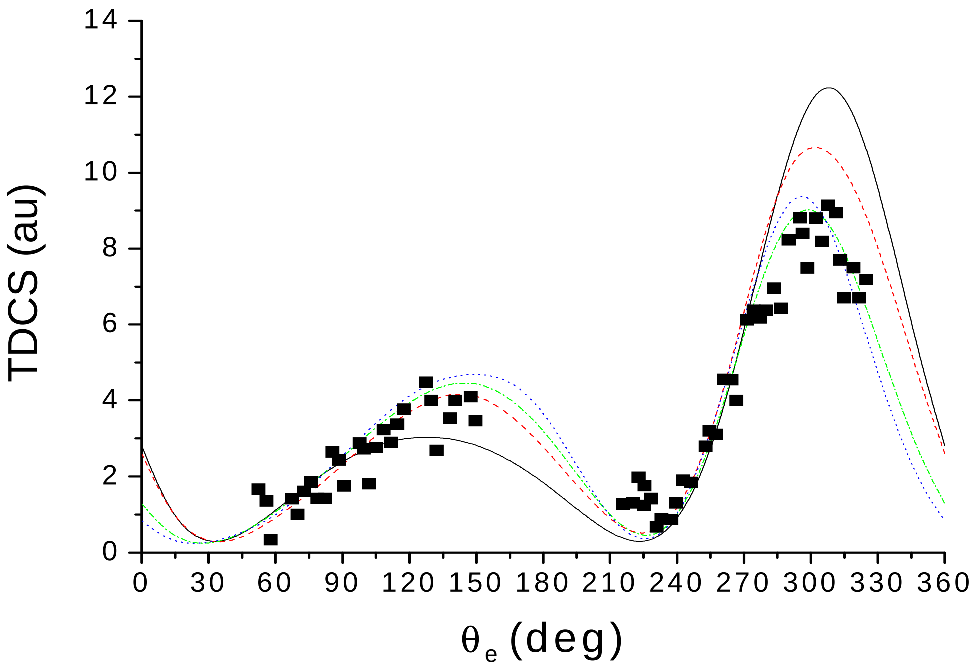
360
θe (deg)

Figure 5



TDCS (au)
θe (deg)
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4
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10
12
14
0 30 60 90 120 150 180 210 240 270 300 330 360

Figure 6

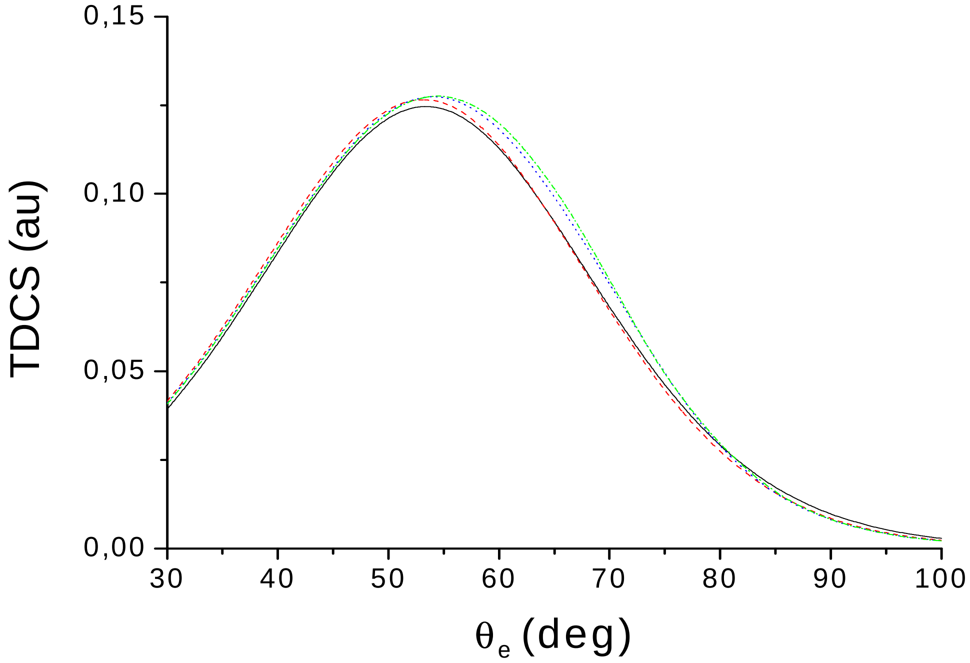


Figure 7a

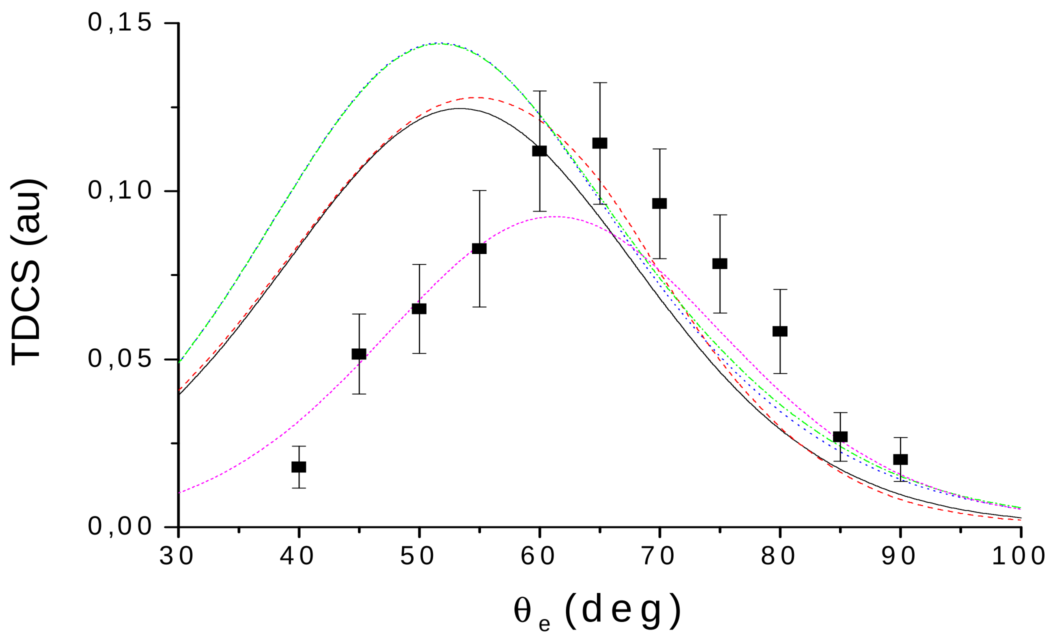


Figure 7b

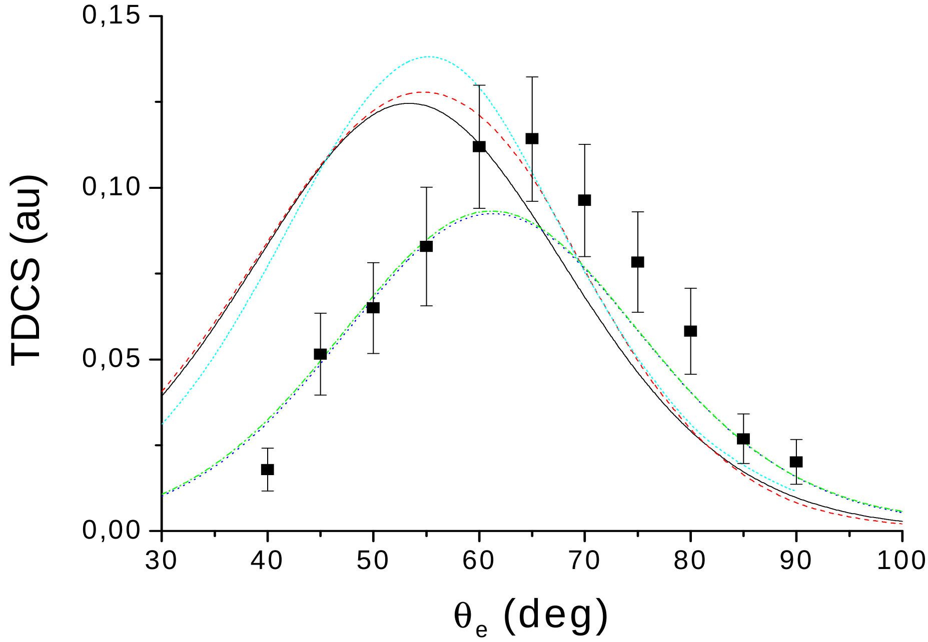


Figure 7c

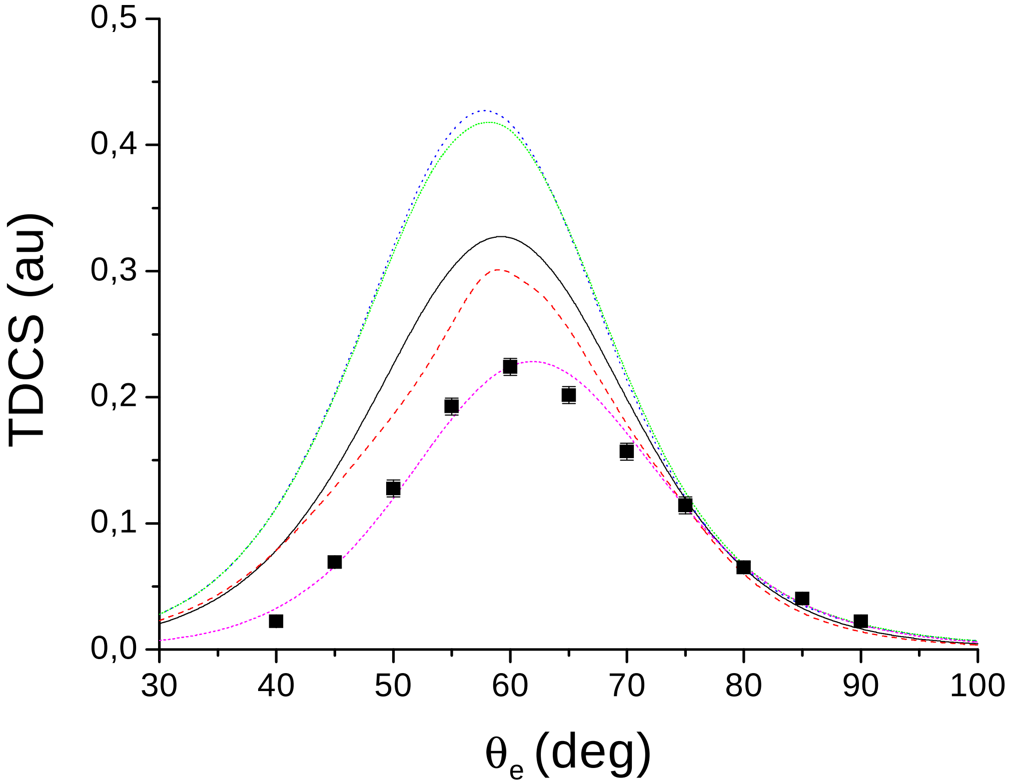


Figure 8a

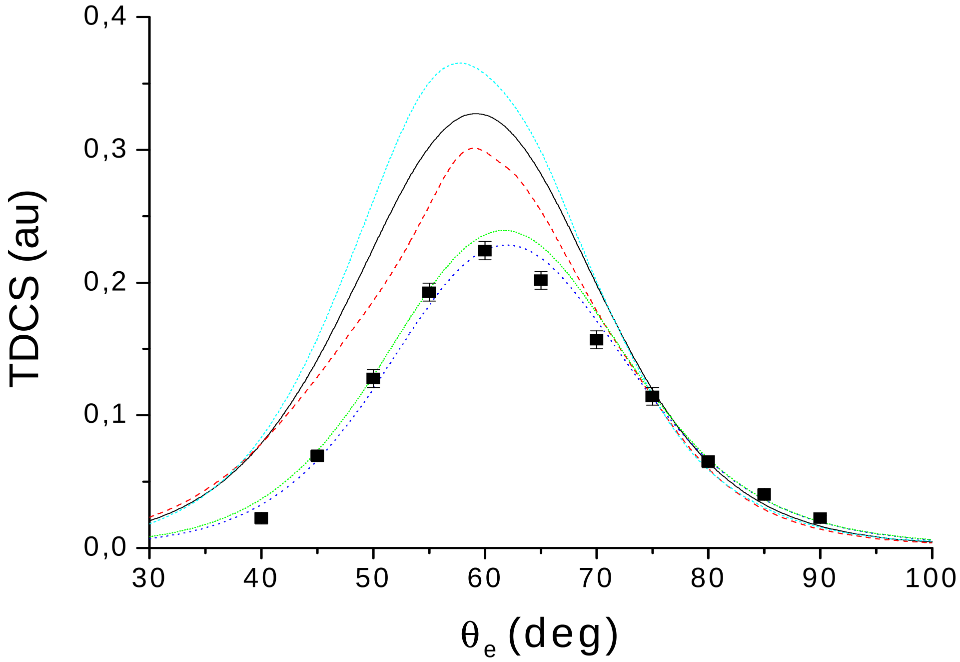
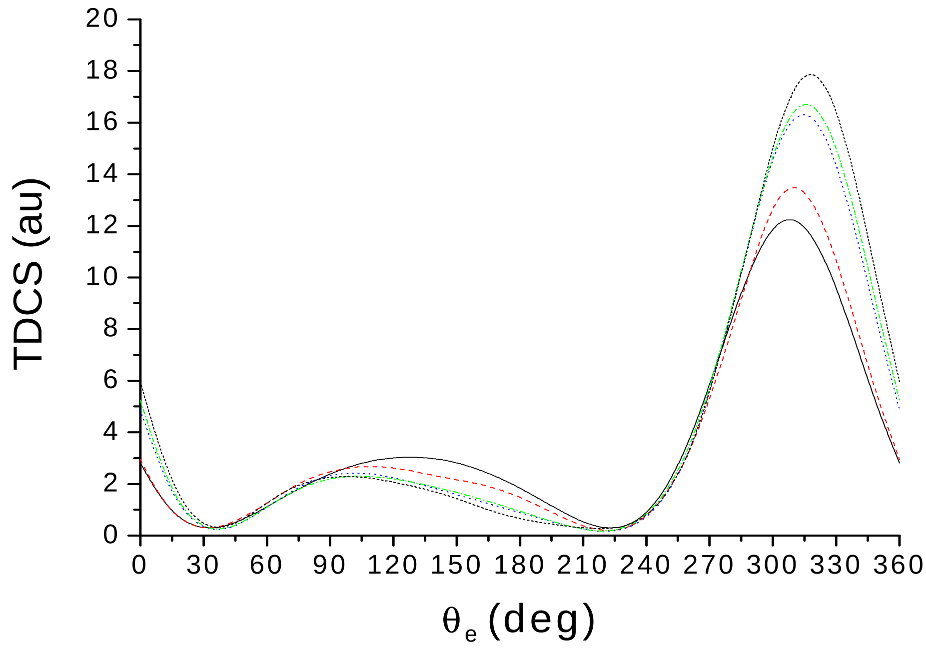


Figure 8b



TDCS (au)
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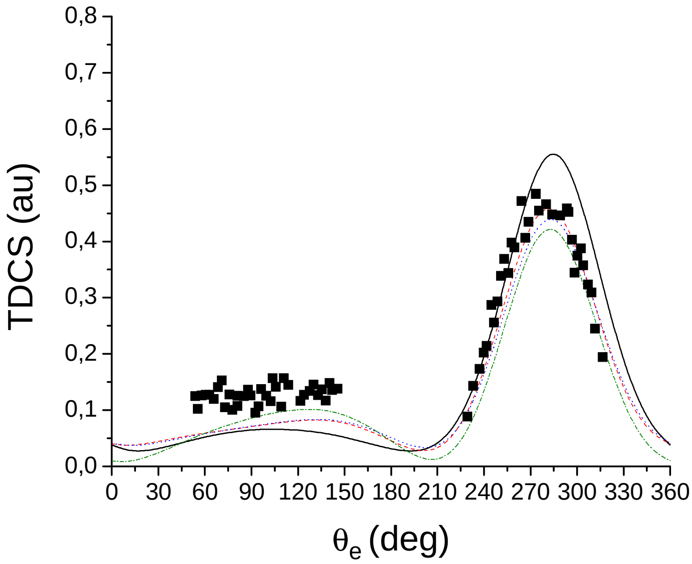
360
θe (deg)

Figure 9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0,4
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0,1
0,0
TDCS (au)
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θe (deg)

Figure 10

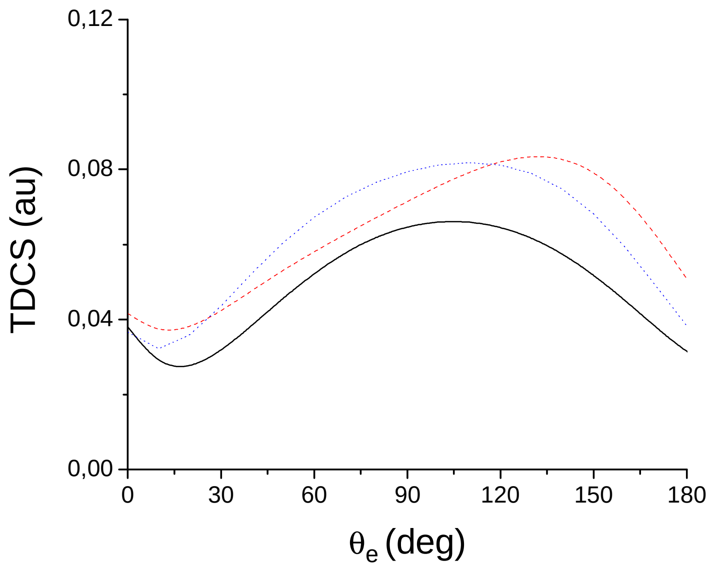
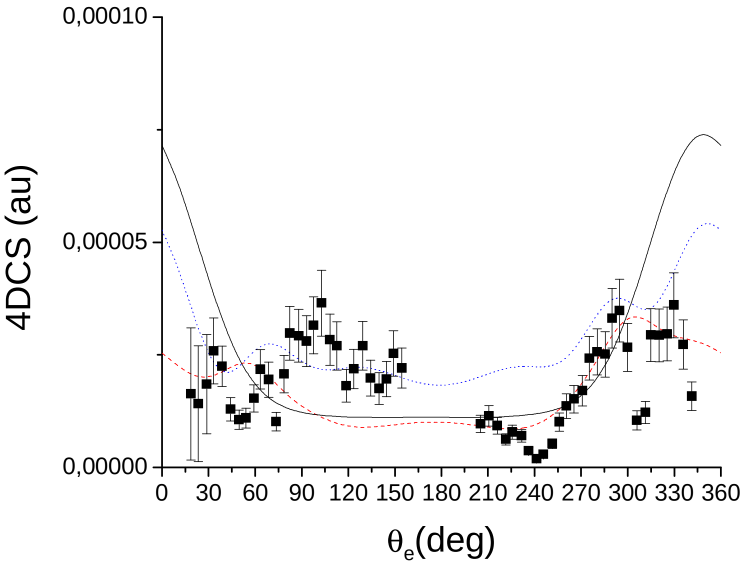


Figure 11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4DCS (au)
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θe(deg)

Figure 12

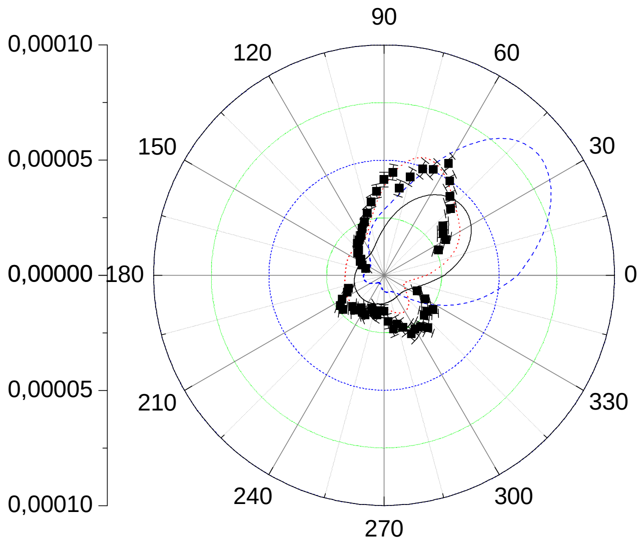

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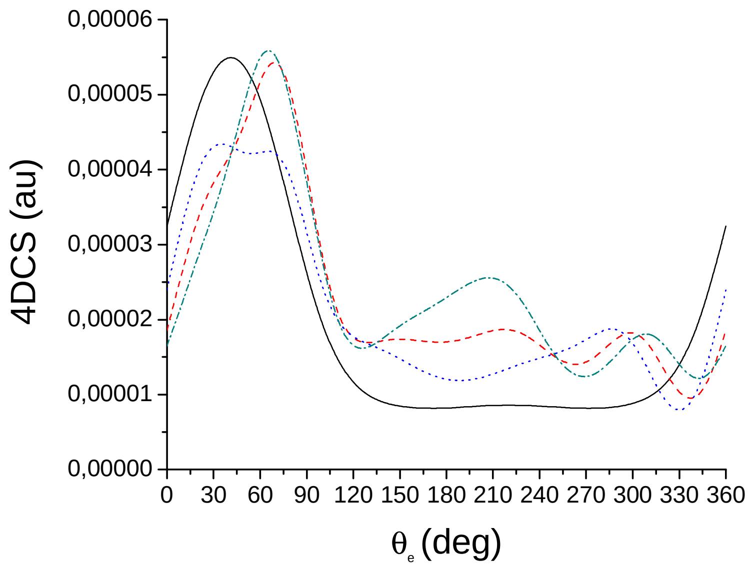
Figure 13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4DCS (au)
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θe (deg)

Figure 14