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# Triple differential cross sections for ionization of hydrogen atoms by positrons in a Schwinger variational calculation

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**Abstract.** Schwinger variational principle has been used to calculate triple differential cross-sections for ionization of hydrogen atoms by positrons at intermediate and high energies for Ehrhardt type asymmetric geometry. The results agree in general with the calculations of Brauner *et al* [8] and with the second Born calculation.

**Keywords.** Cross section; collision; ionization; peak; scattering.

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## 1. Introduction

The study of ionization collisions of atoms by incident charged particles has been an active field of research for the past few decades. Much emphasis has been laid on the study of triple differential cross sections (TDCS) for ionization of atoms by electrons. These studies focus light on various aspects of the ionization problem. In this connection the theoretical work of Byron *et al* [1, 2], Curran and Walters [3] and Curran *et al* [4], Schlemmer *et al* [5], Jones *et al* [6], McCarthy *et al* [7], Brauner *et al* [8], Das and Seal [9, 10] and Seal and Das [11] and the experimental works of Ehrhardt *et al* [12], Ehrhardt [13] and Lohmann *et al* [14] are noteworthy.

For a long time it has been known that positron is more efficient in ionization of atoms and molecules. Recent measurements of total cross sections for hydrogen atoms [15] and hydrogen molecules [16] by positron impact further confirm this. TDCS measured results for positrons are not available now. However, in near future, when such results will be available a new dimension will be added to the ionization studies. A few calculations for total cross sections for ionization of hydrogen atoms by positrons exist at present [17–20]. Brauner *et al* [8] also recorded TDCS results for ionization of hydrogen atoms by positrons along with those for ionization by electrons.

Recently we have made a Schwinger variational calculation (SVC) of TDCS for ionization of hydrogen atoms by electrons and obtained good results [21]. Here we want to report our TDCS results in certain cases for ionization by positrons obtained with the same variational method.

## 2. Schwinger variational principle

Schwinger variational principle for the *T*-matrix elements may be written as (see

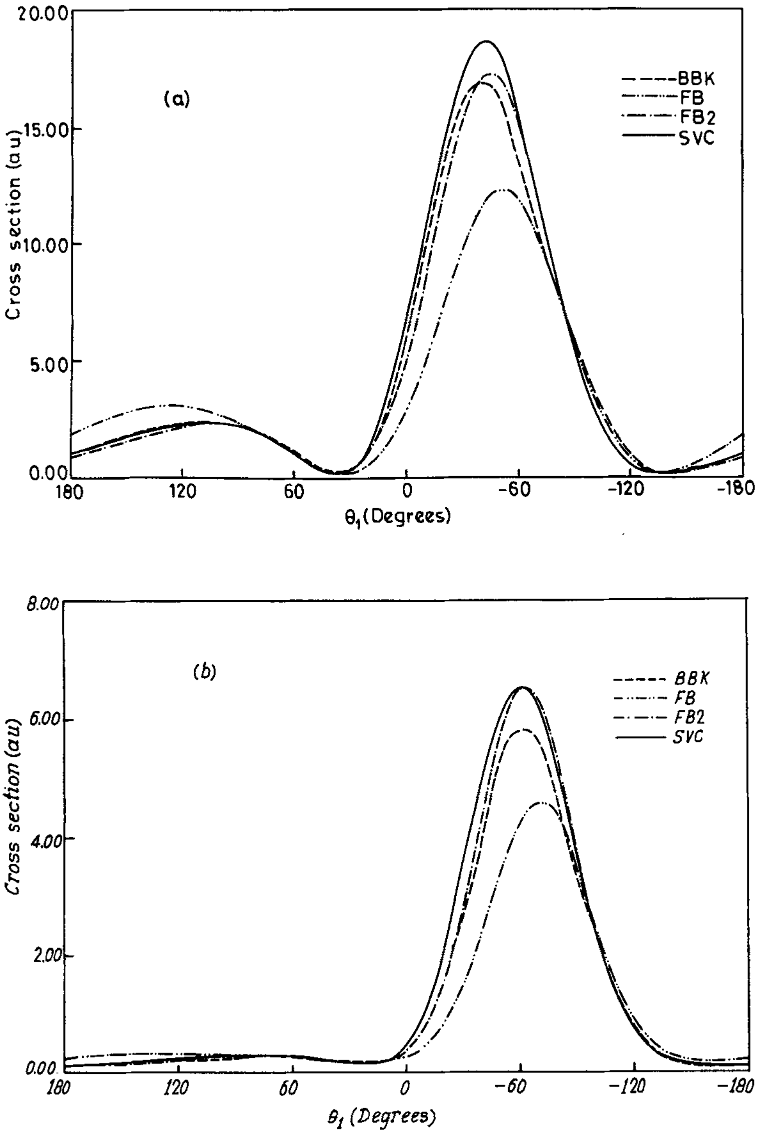

**Figure 1.** TDCS versus ejection angle $\theta_1$ for ionization of hydrogen atoms by positrons at $E_i = 250\,\text{eV}$, $E_1 = 5\,\text{eV}$, $\theta_1 = 3°$ (**a**) $\theta_2 = 8°$ (**b**). Theory: —— present results (SVC); - - - - - results of Brauner *et al* (BBK); —·— FB2; —··— FB.

Joachain [22])

$$[T] = \frac{\langle \Phi_f | V | \Psi_i^+ \rangle \langle \Psi_f^{(-)} | V | \Phi_i \rangle}{\langle \Psi_f^{(-)} | V - VG^{(+)} V | \Phi_i \rangle}. \tag{1}$$

It is easily checked that this is stationary (to 1st order) under arbitrary variations

$$|\Psi^{(\pm)}\rangle \rightarrow |\Psi^{(\pm)}\rangle + \Delta |\Psi^{(\pm)}\rangle.$$

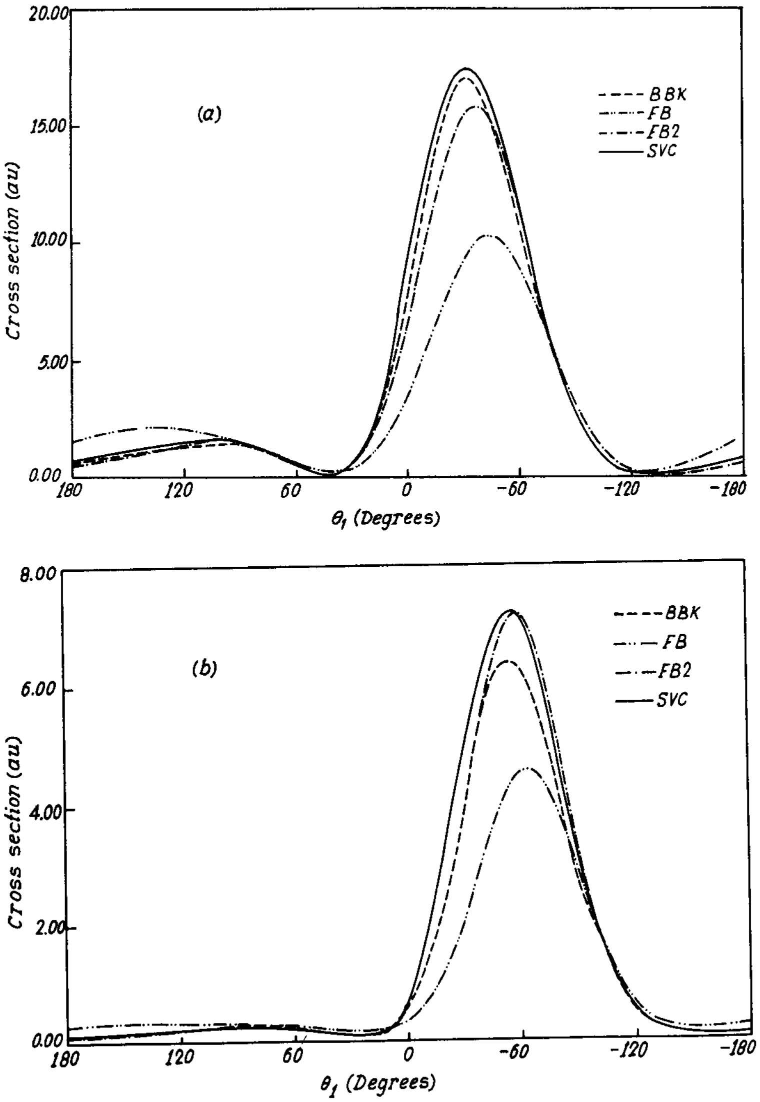

**Figure 2.** Same as figure 1 except for $E_i = 150\,\mathrm{eV}$, $E_1 = 5\,\mathrm{eV}$, $\theta_2 = 4°$ (**a**) and $\theta_2 = 10°$ (**b**).

This provides the variational principle. Here $|\Phi_i\rangle$ and $|\Phi_f\rangle$ are unperturbed initial and final states, $|\Psi_i^{(+)}\rangle$ and $|\Psi_f^{(-)}\rangle$ are the initial and final channel exact states respectively. $V$ is the interaction potential and $G^{(+)}$ is the Green's function for the perturbed Hamiltonian in which the interaction $V$ is omitted. It is reasonable at high energies to approximate $|\Psi_i^{(+)}\rangle$ and $|\Psi_f^{(-)}\rangle$ by $|\phi_i\rangle$ and $|\Phi_f\rangle$ respectively. The resulting scattering amplitude is then given by

$$f = \frac{f_B \cdot f_B}{f_B - f_{B2}}. \tag{2}$$

When $f_{B2}$ is small compared to $f_{\mathrm{B}}$,

$$f \approx f_{\mathrm{B}} + f_{\mathrm{B}2}, \tag{3}$$

the second Born amplitude.

The present calculation is effectively same as our recent work [21] except for a change in sign in the interaction potential.

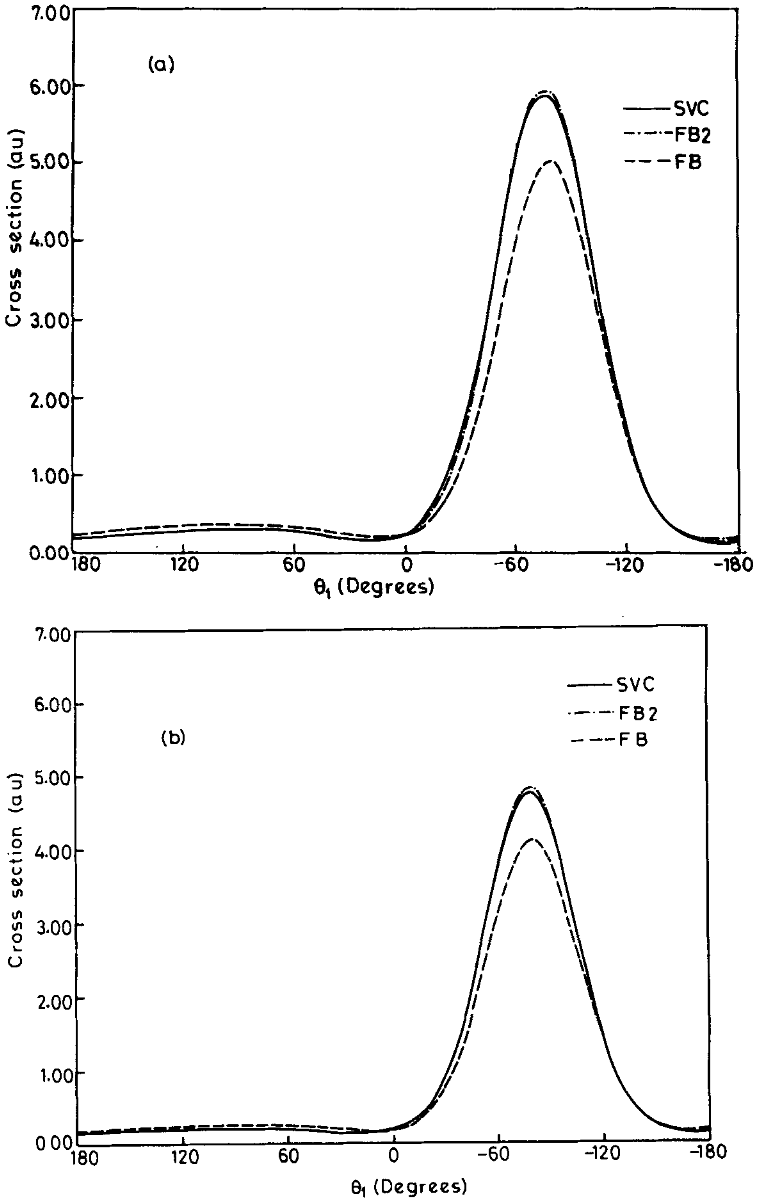

**Figure 3a, b.**

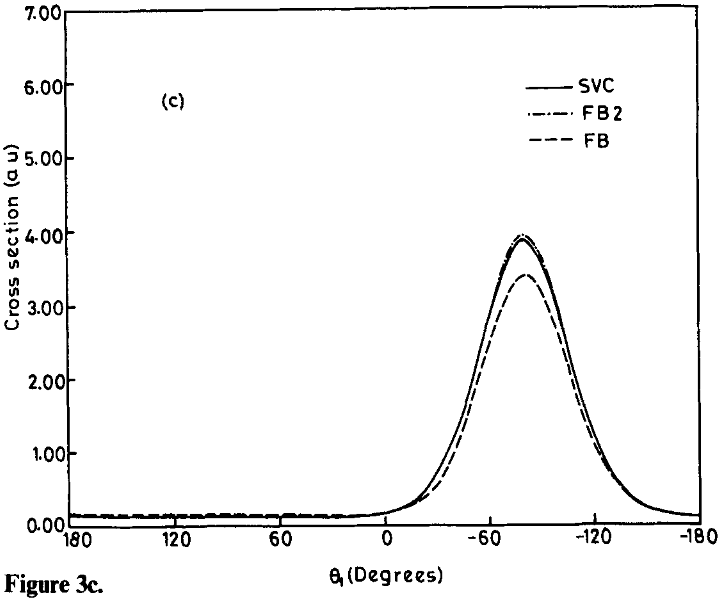

**Figure 3c.**

**Figure 3.** As in figure 1 with $E_1 = 5\,\text{eV}, \theta_2 = 5°, E_i = 600\,\text{eV}$ (a), $E_i = 800\,\text{eV}$ (b) and $E_i = 1000\,\text{eV}$. Theory — SVC; —·— FB2; — — — FB.

## 3. Results and discussion

We have used here the usual notations: $E$ for energy, $p$ for momentum, $\theta$ for scattering angle (referred to incident particle momentum direction as polar axis). $E_i, p_i$ refer to the incident particle, $E_1, p_1, \theta_1$ to the ejected particle and $E_2, p_2, \theta_2$ to the scattered particle. The scattering is considered in a plane.

Three representative sets of results are presented in figures 1(a), 1(b), 2(a), 2(b) and 3(a), 3(b), 3(c) respectively. Figures 1(a) and 1(b) correspond to $E_i = 250\,\text{eV}, E_1 = 5\,\text{eV}, \theta_2 = 3°$ (1(a)) and $\theta_2 = 8°$(1(b)). In figures 2(a) and 2(b) $E_i = 150\,\text{eV}, E_1 = 5\,\text{eV}, \theta_2 = 4°$ (2(a)) and $\theta_2 = 10°$, (2(b)), while in figures 3(a), 3(b) and 3(c), $E_1 = 5\,\text{eV}$, $\theta_2 = 5°$; $E_i = 600\,\text{eV}$ (3(a)), $E_i = 800\,\text{eV}$ (3(b)), $E_i = 1000\,\text{eV}$ (3(c)).

As no experimental data for positron impact ionization are available, we compare our results with the theoretical results of Brauner *et al* [8] (see figures 1 and 2), second Born approximation (FB2) and the first Born approximation (FB). At intermediate energies (150 eV–200 eV), the agreement of the present results (SVC) with FB2 and those of Brauner *et al* are fairly good. Since these three results agree well, we may conclude that first Born approximation underestimates cross section in the binary peak region. This is plausible because it is a high energy approximation.

At high energies (600 eV, 800 eV, 1000 eV presented in figures 3) the present results and FB2 results agree remarkably. There is practically no difference between these two. Even at 1000 eV the first Born approximation results differ significantly from that of FB2 and the present results in the binary peak region, though a very slow convergence to the SVC results from 600 eV to 1000 eV is detectable. In the recoil peak region first Born approximation seems to work much better at these energies.

Certain points need to be noted for the present results. Binary peaks are shifted to smaller angles compared to first Born results and the peak heights are much larger. These are just opposite for ionization by electrons. The recoil peak heights are smaller for ionization by positrons compared to those by electrons. At large momentum transfers the present results tend to depart from those of Brauner *et al* [8].

## 4. Conclusions

It is interesting to note the good agreement between the Schwinger variational results and those of Brauner *et al.* However, at large momentum transfers these tend to depart from each other. Future experimental confirmation or otherwise of these results will be interesting. Schwinger variational calculation for ionization of hydrogen and helium atoms by electrons and positrons using more accurate wave functions such as that used by Das and Seal [9] may produce better results.

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