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Schwinger variational calculation of ionization of hydrogen atoms for large momentum transfers

K CHAKRABARTI
Department of Mathematics, Scottish Church College, 1 & 3 Urquhart Square,
Kolkata 700 006, India

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Abstract. Schwinger variational principle is used here to study large momentum transfer cases of electron and positron impact ionization of atomic hydrogen from the ground state at intermediate and moderately high energies. The results appear somewhat better compared to other theories.

Keywords. Variational principle; ionization; cross section.

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1. Introduction

The description of the ionization of atomic hydrogen in the intermediate and high energy range has attracted a lot of attention. The dynamics of this (e, $2e$) reaction has been investigated in a wide variety of kinematic conditions experimentally as well as theoretically. In the intermediate energy range and small momentum transfers Ehrhardt type asymmetric geometries have been widely used to study the kinematics (for a review see Ehrhardt *et al* [1]). The Ehrhardt type kinematics are characterized by small momentum transfers to the target. On the other hand, symmetric geometries characterized by nearly equal energy partitioning and nearly equal emergence angles, have also been used. Such experiments have been performed by Weigold *et al* [2], Weigold and McCarthy [3], Pochat *et al* [4, 5].

The theoretical description of ionization in the intermediate and high energy range have been done earlier using a first or second Born approximation and its variants by Byron *et al* [6–9]. Non perturbative approaches with asymptotically correct wave functions have been used by Brauner *et al* [10,11], Berakdar [12]. Das and Seal [13] used a multiple scattering approach to the problem and obtained very good results in the intermediate energy range for a wide variety of kinematic conditions. Close coupling calculations like the CCC calculation of Bray *et al* [14] have also been used very successfully. We also mention that there are numerous DWBA approaches to these problems.

Earlier we had used Schwinger variational principle (Das *et al* [15,16]) to study ionization in the intermediate energy range. We were motivated by the fact that variational principles often produce very accurate results if good trial functions are used. Also our choice of unperturbed initial and final channel states as trial functions had made the calculation very simple. We had been able to improve upon the simplified Born approximation (Byron *et al* [7,8]). We also showed that the variational calculation gives better results for larger momentum transfers.

Here we wish to extend our earlier work to large momentum transfer cases at intermediate and moderately high energies. We will show that even for large momentum transfers simple trial functions are capable of producing results which are comparable to, sometimes even better than, other available theories.

2. Schwinger variational principle

For direct collisions (i.e. when there are no rearrangements) Schwinger variational principle for the T-matrix can be written as [17]

$$[T] = \frac{\langle \Phi_{\mathrm{f}} | V | \Psi_{\mathrm{i}}^{(+)} \rangle \langle \Psi_{\mathrm{f}}^{(-)} | V | \Phi_{\mathrm{i}} \rangle}{\langle \Psi_{\mathrm{f}}^{(-)} | V - V G_{\mathrm{i}}^{(+)} V | \Psi_{\mathrm{i}}^{(+)} \rangle}. \tag{1}$$

Here Φ_{i} and Φ_{f} are unperturbed but asymptotically correct eigenstates of the hamiltonian in the initial and final channels; $\Psi_{\mathrm{i}}^{(+)}$ and $\Psi_{\mathrm{f}}^{(-)}$ are the exact eigenstates of the hamiltonians in the initial and final channels satisfying outgoing and incoming wave boundary conditions. $G_{\mathrm{i}}^{(+)}$ is the Green's function for hamiltonian in the initial channel and V is the corresponding perturbation. It can be easily shown that the expression (1) for the T-matrix is stationary under arbitrary variations

$$|\Psi_{\mathrm{i,f}}^{(\pm)}\rangle \to |\Psi_{\mathrm{i,f}}^{(\pm)}\rangle + \Delta |\Psi_{\mathrm{i,f}}^{(\pm)}\rangle. \tag{2}$$

At intermediate and high energies the trial functions $\Psi_{\mathrm{i}}^{(+)}$ and $\Psi_{\mathrm{f}}^{(-)}$ can be reasonably approximated by the unperturbed states Φ_{i} and Φ_{f}. The accuracy of the computed cross sections would increase with a better choice of the trial functions, however, the simple choice of unperturbed states as trial functions appears to give good results in the energy range and kinematic conditions we consider here. After replacing $\Psi_{\mathrm{i}}^{(+)}$ and $\Psi_{\mathrm{f}}^{(-)}$ with Φ_{i} and Φ_{f} the direct scattering amplitude can be written as

$$f_{\mathrm{d}} = \frac{f_{\mathrm{B}} \cdot f_{\mathrm{B}}}{f_{B} - f_{\mathrm{B2}}}, \tag{3}$$

where f_{B} is the first Born scattering amplitude and f_{B2} is the second term in the Born series for the scattering amplitude. It is interesting to note that the result also follows as a Padé approximant to the scattering amplitude (see for example [18] and references therein). Retaining terms up to second order we can write,

$$\begin{aligned} f_{\mathrm{d}} &\approx f_{\mathrm{B}} + f_{\mathrm{B2}} \\ &= f_{\mathrm{B}}(1 + f_{\mathrm{B2}}/f_{\mathrm{B}}) \\ &\approx \frac{f_{\mathrm{B}}}{1 - f_{\mathrm{B2}}/f_{\mathrm{B}}} \\ &= \frac{f_{\mathrm{B}} \cdot f_{\mathrm{B}}}{f_{\mathrm{B}} - f_{\mathrm{B2}}} \end{aligned} \tag{4}$$

which agrees with expression (3) calculated using the variational principle.

Evaluation of f_{B} is straightforward (see [9]). For f_{B2} we use a simplified second Born approximation of Byron *et al* [6] and evaluate it using the closure approximation, as in our previous work.

3. Results

The experimental results with which we compare our results are not absolute. However, in our earlier work we compared our results with the absolute experimental data of Ehrhardt *et al* [1] and Ehrhardt [19] and obtained very good agreement. So we believe that our results give reasonably correct absolute cross sections. Therefore we normalize the experimental values with our results by multiplying each set of data with a single factor.

Figure 1 shows results for an incident energy 113.6 eV while the two outgoing electrons have an energy 50 eV each. Two sets of results are presented for $\theta_2 = 35°$ and $\theta_2 = 45°$ with $\phi_1 - \phi_2 = \pi$. These are compared with the DWIA and PWBE results of Weigold *et al* [20] and their relative measurements. The present results appear much better compared with the PWBE and DWIA. The position of the peaks are correctly reproduced after suitable normalization.

In figure 2 we present results for the incident energy 250 eV. The two outgoing electrons have energies 50 eV and 186.4 eV. The figure shows five sets of results corresponding to $\theta_2 = 15°, 20°, 25°, 30°, 35°$ and $\phi_1 - \phi_2 = \pi$. The results are compared with the experimental results of Weigold *et al* [20] and the results of DWIA and PWBE calculations. Our results are in better agreement with the DWIA than with PWBE. At $\theta_2 = 15°$ and $20°$ the PWBE overestimates cross section at the peak whereas both DWBA and the present calculation predict the peak position and peak heights more or less correctly.

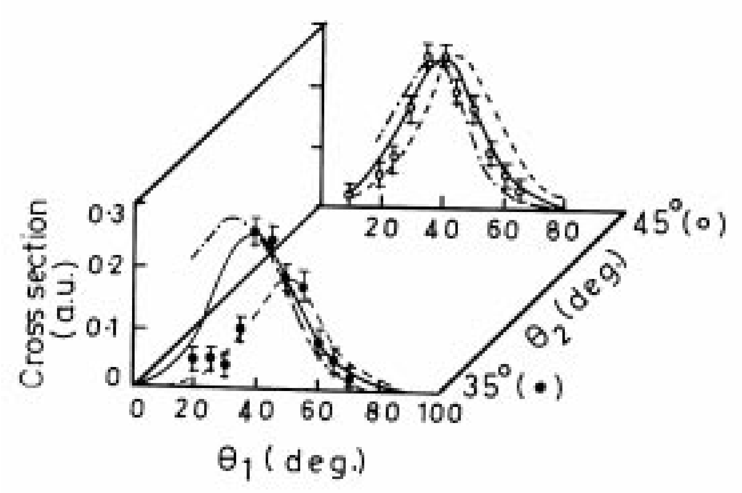

Figure 1. TDCS for ionization of hydrogen atoms by electrons at $E_{\mathrm{i}} = 113.6$ eV, $E_1 = E_2 = 50$ eV, θ_2 being fixed at 35° and 45°, $\phi_1 - \phi_2 = \pi$ and θ_1 variable. *Theory*: Continuous curve – present calculation; dashed curve – DWIA; dash-dotted curve – PWBE. *Experiment*: • (35°), ∘ (45°) Weigold *et al* [20] normalized at $\theta_1 = 40°$, $\theta_2 = 35°$ with the present results.

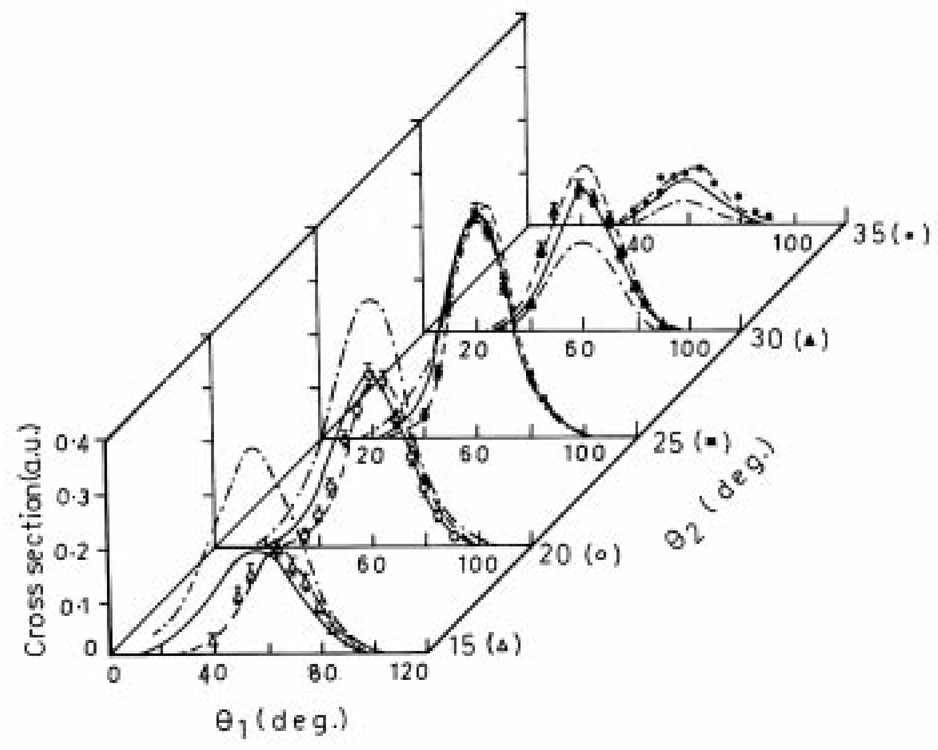

Figure 2. TDCS for ionization of hydrogen atoms by electrons at $E_\mathrm{i} = 250$ eV, $E_1 = 50$ eV, θ_2 being fixed at 15°, 20°, 25°, 30° and 35°, $\phi_1 - \phi_2 = \pi$ and θ_1 variable. *Theory*: Continuous curve, present calculation; dashed curve – DWIA; dash-dotted curve – PWBE. *Experiment*: △ (15°), ○ (20°), ■ (25°), ▲ (30°), • (35°) Weigold *et al* [20] normalized at $\theta_1 = 60°, \theta_2 = 20°$ with the present results.

In figure 3 we display cross sections for an incident energy $E_\mathrm{i} = 413.6$ eV and ejected electron energy $E_1 = 200$ eV. The figure shows three sets of results corresponding to scattering angle $\theta_2 = 30°, 40°, 50°$. We compare the results with the relative measured values of Weigold *et al* [20] and with the theoretical results of DWBA and PWBE. In this case also our results are in good qualitative agreement with the experiments. Quantitatively however, our results appear to be closer to the PWBE results.

Finally in figure 4, cross sections are displayed for an incident energy 413.6 eV, scattering angle $\theta_2 = 30°$ and two different values of ejected electron energy: (a) $E_1 = 50$ eV and (b) $E_1 = 100$ eV. The results are compared with the measured values of Mc Carthy *et al* [21] and with the theoretical results of the second Born approximation (B2), DWBA and DWIA results given in [20]. Except B2 all curves agree in shape. The present results reproduce the experimental data nicely and the height and position of the peak are correctly predicted. Note the pronounced improvement of the variational calculation over the second Born calculation.

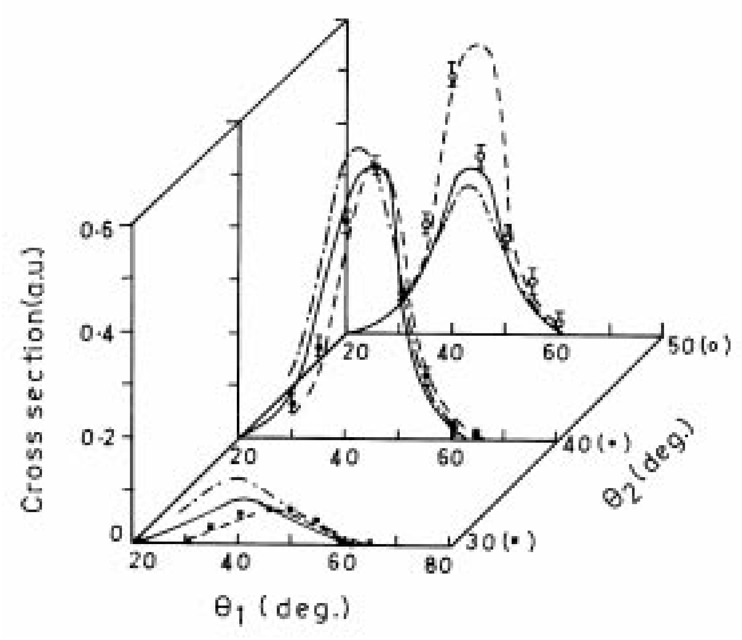

Figure 3. TDCS for ionization of hydrogen atoms by electrons at $E_i = 413.6$ eV, $E_1 = E_2 = 200$ eV, θ_2 being fixed at 30°, 40° and 50°, $\phi_1 - \phi_2 = \pi$ and θ_1 variable. *Theory*: Continuous curve – present calculation; dashed curve – DWIA; dash-dotted curve – PWBE. *Experiment*: ■ (30°), • (40°), ○ (50°) Weigold *et al* [20] normalized at $\theta_1 = 45°$, $\theta_2 = 40°$ with the present results.

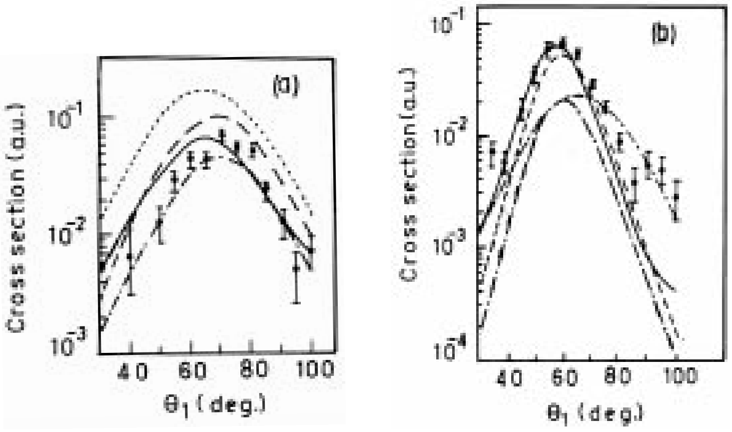

Figure 4. TDCS for ionization of hydrogen atoms by electrons at $E_i = 413.6$ eV, (**a**) $E_1 = 50$ eV, $\theta_2 = 30°$ and (**b**) $E_1 = 100$ eV, $\theta_2 = 30°$ with $\phi_1 - \phi_2 = \pi$ and θ_1 variable. *Theory*: Continuous curve – present calculation; long dashed curve – DWBA; short dashed curve – second Born approximation (SB2); dash-dotted curve – DWIA. *Experiment*: • McCarthy *et al* [21] normalized at a single point in each case.

4. Positron impact ionization at large momentum transfers

It is interesting to see the effect on the cross section when the incident electron is replaced by a positron. Positron impact ionization for small momentum transfers has been studied by Das *et al* [16], Joachain and Piraux [22] and Brauner *et al* [10]. We wish to make a brief study of this ionization process for large momentum transfers. To the best of our knowledge this has not been done before. Since there is no experimental data available we compare our results with the TDCS for electron impact ionization and the first Born TDCS.

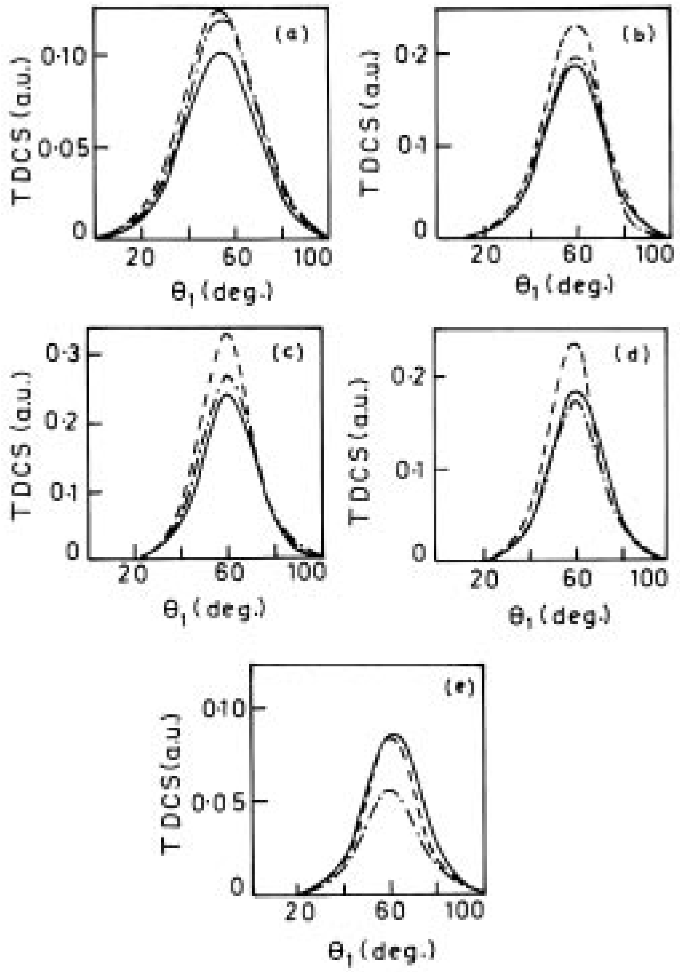

Figure 5. TDCS for ionization of hydrogen atoms by positrons at $E_i = 250$ eV, $E_1 = 50$ eV and (**a**) $\theta_2 = 15°$, (**b**) $\theta_2 = 20°$, (**c**) $\theta_2 = 25°$, (**d**) $\theta_2 = 30°$, (**e**) $\theta_2 = 35°$, $\phi_1 - \phi_2 = \pi$ and θ_1 variable. *Theory*: Continuous curve – present calculation; dashed curve – first Born results for positron; dash-dotted curve – present results for electron.

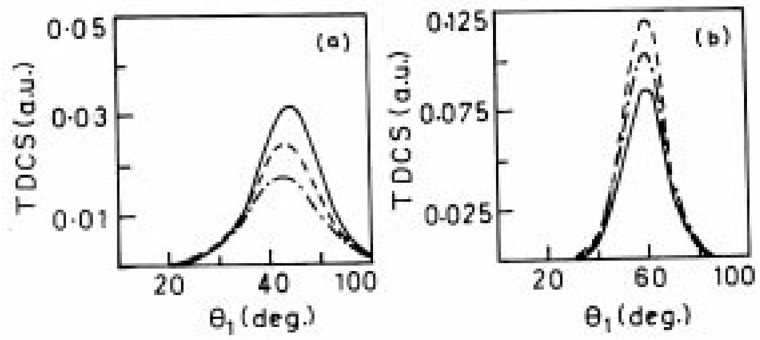

Figure 6. Same as figure 5 except for $E_i = 413.6$ eV, $\theta_2 = 30°$ and (**a**) $E_1 = 50$ eV and (**b**) $E_1 = 100$ eV.

Five sets of results are presented in figure 5 where the incident energy is 250 eV, ejected electron energy 50 eV and positron scattering angles: (a) $\theta_2 = 15°$, (b) $\theta_2 = 20°$, (c) $\theta_2 = 25°$, (d) $\theta_2 = 30°$ and (e) $\theta_2 = 35°$. The noteworthy feature is the smallness of the TDCS for incident positrons compared to the TDCS for incident electrons for smaller scattering angles (figures 5a, 5b). This is quite contrary to small momentum transfer cases (see [23] for example). The trends are reversed for larger scattering angles (figures 5d, 5e), where the TDCS for incident positrons are larger.

Figure 6 shows two results for an incident energy 413.6 eV, scattering angle $\theta_2 = 30°$ and ejected electron energy $E_1 = 50$ eV (figure 6a) and $E_1 = 100$ eV (figure 6b). From figures 6a and 6b it is clear that for fixed positron scattering angle θ_2, the peak height of the TDCS for incident positrons is greater than that for incident electrons for larger momentum transfers to the target.

Except in figure 5c, for an incident energy 250 eV and scattering angle $\theta_2 = 35°$, the first Born cross section never agrees with the variational calculation. The first Born TDCS also appears to be generally larger than that of the present calculation. This is in disagreement with our earlier findings for small momentum transfer cases (see [15]).

5. Conclusion

In this work we have used Schwinger variational principle to study electron impact ionization of atomic hydrogen at intermediate and moderately high energies. Our results appear a little better compared to other theories. Positron impact ionization is also considered briefly to see the differences. The variational calculation is also very simple. The method can be improved by using better trial functions.

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