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Schwinger Variational Calculation for Ionisation of Hydrogen Atoms by Electrons

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Abstract

The Schwinger variational principle has been used to calculate the triple differential cross section for ionisation of hydrogen atoms by electrons at intermediate and high energies for Ehrhardt-type asymmetric geometry. The results are somewhat better in the recoil peak regions compared with those of the second Born and other similarly successful calculations. The binary and recoil peaks are almost exactly reproduced in the present calculation.

1. Introduction

The study of electron–atom ionisation collisions at intermediate and high energies is now an active field of research. Many theories have been advanced for these problems, but our knowledge is still far from complete. Among the theories now used to describe the triple differential cross section (TDCS) for Ehrhardt-type asymmetric geometry, that by Brauner *et al.* (1989) is particularly noteworthy. Qualitatively, this describes the TDCS results in the above kinematic domain very satisfactorily. However, there are gross quantitative differences (see Das and Seal 1993). Quantitatively, the experimental results of Ehrhardt and associates (Ehrhardt 1991; Ehrhardt *et al.* 1986) are well described by many calculations, such as the second Born approximation (B2) (Byron *et al.* 1980), the eikonal Born series method (EBS) (Byron *et al.* 1983), the pseudo-state close coupling calculation (PSCC) (Curran and Walters 1987; Curran *et al.* 1991), the CB2 calculation (Schlemmer *et al.* 1991), the 3DWBA calculation (Jones *et al.* 1993), and the multiple scattering calculation (Das and Seal 1993; Seal and Das 1994). However, despite continuous efforts made to reproduce exactly the experimentally observed results, there are still certain gaps to be filled. In particular, all the above theories under-estimate the cross section in the recoil peak region, particularly for large momentum transfer in the Ehrhardt kinematic domain.

Now it is well known that variational principles, if suitably applied, can give very accurate results. As far as we know, variational principles have not been used in the study of ionisation problems. Schwinger variational principles are particularly noteworthy. We propose here to make use of these principles in a study of the TDCS results for certain cases in the Ehrhardt kinematic domain.

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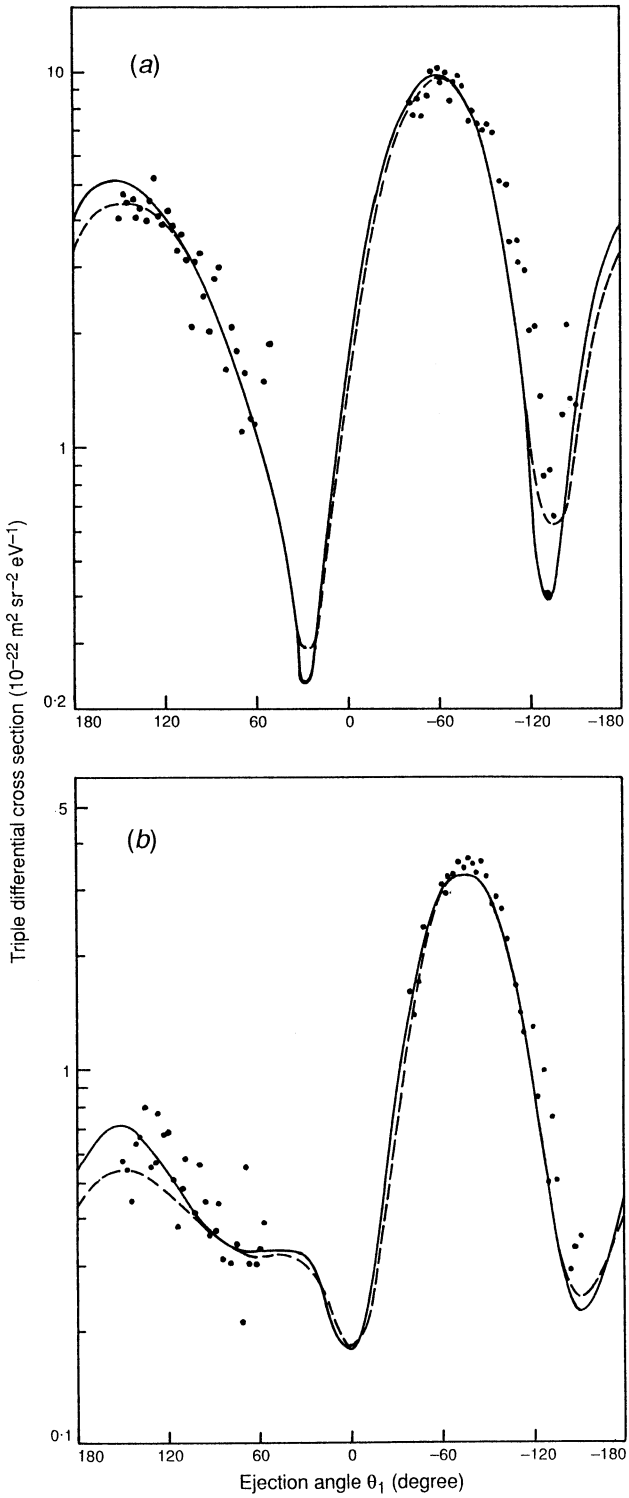

Fig. 1. TDCS versus ejection angle θ_1 for ionisation of hydrogen atoms by electrons at $E_i = 250$ eV and $E_1 = 5$ eV and for (*a*) $\theta_2 = 3°$ and (*b*) $\theta_2 = 8°$. Present theory, solid curve; (simplified) second Born approximation, dashed curve; and experiment, Ehrhardt (1991) and Ehrhardt *et al.* (1986).

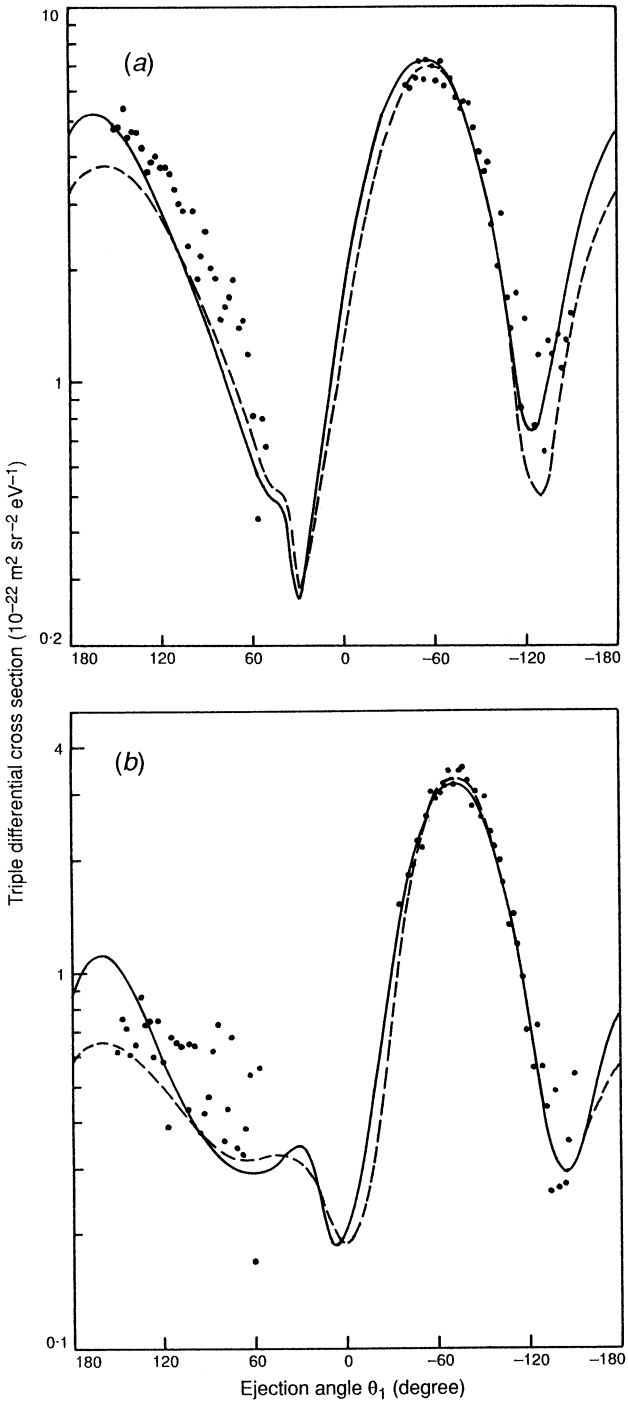

Fig. 2. As for Fig. 1, except for $E_i = 150$ eV and $E_1 = 5$ eV and for (*a*) $\theta_2 = 4°$ and (*b*) $\theta_2 = 10°$.

2. Schwinger Variational Principle

The Schwinger variational principle for the direct T-matrix element for electron–hydrogen ionisation collisions may be written as (see Joachain 1979)

$$[T] = \frac{\langle \Phi_f | V_d | \Psi_i^{(+)} \rangle \langle \Psi_f^{(-)} | V_d | \Phi_i \rangle}{\langle \Psi_f^{(-)} | V_d - V_d G_d^{(+)} V_d | \Phi_i \rangle}, \tag{1}$$

where $|\Phi_i\rangle$ and $|\Phi_f\rangle$ are unperturbed initial and final states, $|\Psi_i^{(+)}\rangle$ is the initial channel exact state, $|\Psi_f^{(-)}\rangle$ is the final channel exact state, V_d is the interaction potential for direct scattering and $G_d^{(+)}$ is Green's function for the perturbed Hamiltonian in which the interaction V_d is omitted. It is reasonable for intermediate and 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

$$f_d = \frac{f_B^2}{f_B - f_{B2}}. \tag{2}$$

Here f_B is the first Born amplitude and f_{B2} the second order term in the Born series. If f_{B2} is small compared with f_B, then an expansion of $(f_B - f_{B2})^{-1}$ in (2) may be made in the form $f_B^{-1}(1 + f_{B2}/f_B + \ldots)$ leading to the second Born approximation

$$f_d = f_B + f_{B2}. \tag{3}$$

However, generally it is desirable to keep the full expression (2). In this paper we use (2) to compute the TDCS results for Ehrhardt-type kinematical conditions. As usual we neglect exchange effects.

Regarding notation we add that E_i, p_i refer to the incident electron, E_1, p_1, θ_1 to the 'ejected' electron and E_2, p_2, θ_2 to the scattered electron. The scattering takes place in a plane and E stands for energy, p for momentum and θ for the scattering angle (referred to the incident electron momentum direction as the polar axis). To calculate f_{B2} we follow Byron *et al.* (1980) and use a closure approximation and then integrate the resultant three-dimensional integral numerically.

3. Results and Discussion

We have applied the Schwinger variational principle in the calculation of the TDCS results for ionisation of hydrogen atoms by electrons at intermediate and high energies for Ehrhardt kinematic conditions. Two representative sets of results are presented in Figs 1 and 2. Fig. 1 corresponds to $E_i = 250$ eV, $E_1 = 5$ eV and $\theta_2 = 3°$ and $8°$, while Fig. 2 corresponds to $E_i = 150$ eV, $E_1 = 5$ eV and $\theta_2 = 4°$ and $10°$. We have presented the results in a logarithmic plot, which gives an enlarged view of that region where cross sections are small. Moreover, the percentage errors at different points can be estimated directly from such a plot. Here we compare our results with the measured values of Ehrhardt and associates (Ehrhardt 1991; Ehrhardt *et al.* 1986) and with the theoretical results of the second Born approximation, only for the reason that other calculations

for these kinematic conditions give good but very similar results. The present results agree nicely with experiment and with the B2 results in the binary peak region. There are slight departures, however, beyond $-120°$. In the recoil peak region there is also good agreement for very small momentum transfers (see Figs 1*a* and 2*a*). For slightly larger momentum transfers there are considerable differences between the present and B2 results. Here B2 underestimates the cross section but our results agree nicely with the measured values (scatter in the experimental values makes the comparision difficult). The recoil peak heights are almost exactly reproduced in this calculation. For larger momentum transfers the cross sections in the recoil peak region are about 30% higher than for B2 (see Figs 1*b* and 2*b*). Thus the present calculation gives significantly improved results in the recoil peak region (on a linear scale agreement with experiment would appear much better). The higher order effects of the interaction which are implicitly included in the variational formula are responsible for the improvement.

The results for 250 eV are a little better compared with those for 150 eV for the obvious reason that the approximate trial functions are more accurate for higher energies. For much lower energies, such as 54·4 eV, the calculated results are even worse than for the second or first Born approximations, a characteristic feature of variational calculations—a bad wavefunction leads to poor results.

4. Conclusions

Schwinger variational principles are successful in describing events for Ehrhardt-type asymmetric geometry in the case of ionisation of hydrogen atoms by electrons at intermediate and high energies. In fact, compared with all other theories proposed so far, this approach provides the best description of the TDCS results under Ehrhardt kinematic conditions. The same may be true for ionisation of other atoms as well. Its success or otherwise remains to be seen for other kinematic conditions.

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