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# Distorted-wave Born Approximation for the Ionisation of Hydrogen by Electrons

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*Abstract*

Matrix elements for ionisation play an important part in electron-atom scattering calculations. Two methods for describing ionisation that can be incorporated into a scattering calculation are tested here against coplanar asymmetric experimental differential cross sections at 150 and 250 eV. They are the distorted-wave Born approximation and the coupled pseudostates method. A method that incorporates the exact boundary condition for three charged bodies describes the data significantly better and shows an important direction for improvement of scattering calculations.

## 1. Introduction

The distorted-wave Born approximation (DWBA) plays a central role in the theory of electron-atom collisions. On the one hand it can be fully implemented in a calculation of the optical potential describing the effect of ionisation on scattering (Bray *et al.* 1989). This contribution is usually important. In many cases the total ionisation cross section is at least a quarter of the total cross section. On the other hand the DWBA has given quite a good description of fully (sometimes called triple) differential experimental cross sections (e.g. Madison *et al.* 1977) and of cross sections with integration over various dimensions of the five-fold kinematic space (e.g. Younger 1980; McCarthy and Zhang 1989).

Because of its role in scattering theory it is essential to test the DWBA as thoroughly as possible in comparison with experiment for the prototype case of hydrogen. It has been somewhat neglected as a serious description of ionisation, possibly because of large numerical errors due to overtruncation of the partial-wave series in early calculations. It is also interesting to test it as a description of ionisation in comparison with other theories, particularly to see if there is a better ionisation theory that could conceivably be implemented in the optical potential for scattering.

We compare three methods of calculating the differential cross section for ionising the hydrogen atom with coplanar asymmetric experimental data at 150 and 250 eV. Two of these methods, the distorted-wave Born approximation (calculated for this work) and the coupled pseudostate method (Curran and Walters 1987) are tractable in a scattering calculation. The third is the only calculation up to the present that includes the exact boundary condition for

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the charged three-body problem (Brauner *et al.* 1989). It has not yet been implemented in a scattering calculation.

## 2. Methods for Treating the Continuum

The first test that must be applied to methods for treating the continuum in scattering calculations is whether they work well for differential ionisation cross sections. This observes the continuum-excitation matrix elements on the energy shell. In this work we consider two basic methods. The first solves a two-body pseudo-problem for the interaction of an electron with a target in a discrete set of states represented by square-integrable functions. The higher-energy states in this problem are not actual eigenstates of any Hamiltonian. They are simply square-integrable functions or pseudostates chosen so that the two-body pseudoproblem represents accurately certain aspects of the real three-body problem. We use as our example the pseudostate ionisation calculation of Curran and Walters (1987).

The second method to be studied here treats the electron-hydrogen problem formally as a three-body problem. We divide the space of target states for our present formal purposes into $P$-space which consists of the discrete states and $Q$-space which is the continuum. The scattering problem for $P$-space (McCarthy and Stelbovics 1980) can be treated by a discrete set of coupled equations for which the potential matrix elements include contributions from the complex polarisation potential, which we write as

$$\langle \mathbf{q}'i \mid V_S^{(Q)} \mid j\mathbf{q}\rangle = \int d^3k' \int d^3k \langle \mathbf{q}'i \mid \Psi_S^{(-)}(\mathbf{k}',\mathbf{k})\rangle \frac{1}{E^{(+)} - \frac{1}{2}(k'^2 + k^2)} \times \langle \Psi_S^{(-)}(\mathbf{k}',\mathbf{k}) \mid V_S \mid j\mathbf{q}\rangle; \quad i,j \in P. \tag{1}$$

Here $\Psi_S^{(-)}(\mathbf{k}',\mathbf{k})$ is the three-body continuum wave function for ingoing spherical-wave boundary conditions and total electron spin $S$, whereas $V_S$ is the appropriate operator for which the corresponding matrix element is the properly-antisymmetrised $T$-matrix element for ionisation. The form of this operator that allows the antisymmetric problem to be treated entirely by the methods of two-body multichannel potential scattering has recently been derived by Stelbovics and Bransden (1989). Ionisation tests the ground-state on-shell combination of matrix elements

$$\frac{d^5\sigma}{d\hat{\mathbf{k}}_A d\hat{\mathbf{k}}_B dE_A} = (2\pi)^4 \frac{k_A k_B}{k_0} \Sigma_S \frac{2S+1}{4} |\langle \Psi_S^{(-)}(\mathbf{k}_A,\mathbf{k}_B) | V_S | 0\mathbf{k}_0\rangle|^2 . \tag{2}$$

This is the differential cross section.

For scattering it has so far proved possible to implement (1) only in the distorted-wave Born approximation (DWBA) in which $\Psi_S^{(-)}(\mathbf{k}',\mathbf{k})$ is approximated by the product of scattering solutions for each electron-ion subsystem (Bray *et al.* 1989):

$$\Psi_S^{(-)}(\mathbf{k}',\mathbf{k}) = \chi^{(-)}(\mathbf{k}')\chi^{(-)}(\mathbf{k}). \tag{3}$$

In this sense the DWBA is again a two-body method. Its advantage compared to the pseudostate method is that it uses exact solutions of the two-body target continuum. Its disadvantage is that it is only an approximate solution of the real continuum problem whereas the pseudostate method is a numerically-exact solution of the pseudoproblem. Comparison with experiment will test how good an approximation to on-shell ionisation is the DWBA and how close the pseudoproblem is to the real three-body problem of on-shell ionisation.

For many years the major difficulty in understanding the target continuum in electron-atom scattering has been the essentially three-body nature of the boundary condition for three charged particles. Recently the exact boundary condition has been established by Brauner *et al.* (1989). They calculated ionisation cross sections using the approximation that the three-body wave function is a product of three functions, one for each two-body subsystem. This approximation would include a factor $\phi(\mathbf{k}'-\mathbf{k})$ in (3), which asymptotically is the correct phase factor for the two-electron subsystem. They showed that this approximate three-body wave function has the correct boundary condition. While this approximation has not yet been incorporated into a calculation of the polarisation potential (1) its value has been assessed in the on-shell ionisation problem. It has proved spectacularly successful in describing relative differential cross sections for coplanar asymmetric ionisation.

## 3. Normalisation of Experimental Cross Sections

It is of course necessary to have absolute experimental cross sections to form a good idea of the validity of a theoretical method. Absolute differential ionisation measurements are very difficult and have only been made on rare occasions (Beaty *et al.* 1977; Stefani *et al.* 1978; van Wingerden *et al.* 1979, 1981).

Two basic methods have been used to put relative measurements on an absolute scale. Both depend to some extent on the validity of the first Born approximation for the double differential cross section. For example Lahmam-Bennani *et al.* (1983) integrate the asymmetric differential cross sections over all directions of the slower electron to estimate the double differential cross section. This is normalised by comparison with measured double differential cross sections put on an absolute scale by using the Bethe sum rule (Lahmam-Bennani *et al.* 1980). The Bethe sum rule is valid if the first Born approximation describes the double differential cross section accurately enough. The other method is to use the optical limit. As the momentum transfer to the fast electron tends to zero the double differential cross section can be simply related to the optical oscillator strength regardless of the validity of the first Born approximation for higher momentum transfer (Inokuti 1971). The optical oscillator strength is obtained from photoionisation measurements. This is the basis of the normalisation method used by Jung *et al.* (1985) and Ehrhardt *et al.* (1986). Avaldi *et al.* (1987) have used a combination of these methods, integrating the differential cross sections to obtain double differential cross sections for comparison with relative double differential cross sections measured as a function of momentum transfer and normalised by extrapolating to the optical limit. Lahmam-Bennani *et al.* (1987) find very good agreement between the three methods.

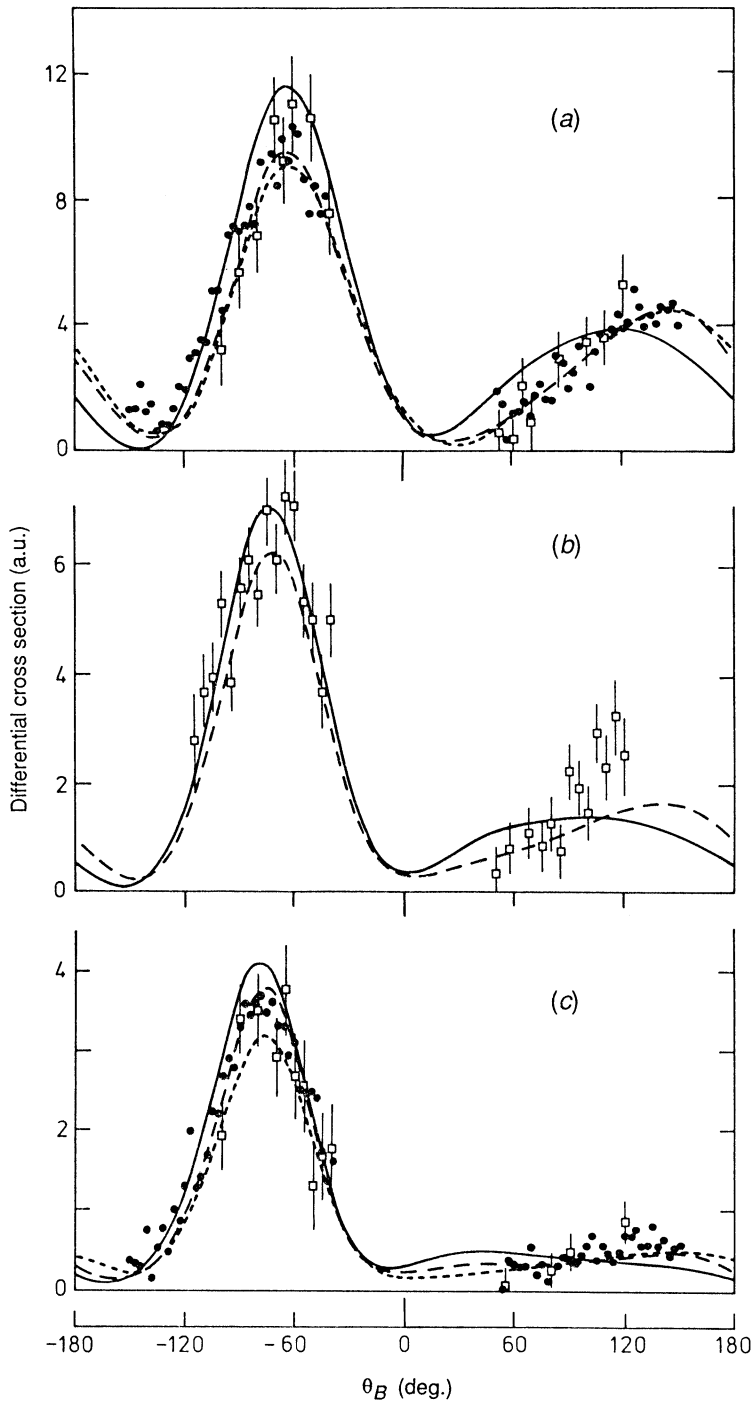


**Fig. 1.** The differential cross section for the ionisation of atomic hydrogen by electron impact. Closed circles: experimental data of Ehrhardt *et al.* (1985, 1986), Klar *et al.* (1987), open squares: experimental data of Lohmann *et al.* (1984), solid curve: DWBA (this work), long dashes: coupled pseudostate method (Curran and Walters 1987), short dashes: calculation incorporating the exact three-body boundary condition (Brauner *et al.* 1989). $E_0 = 250$ eV, $E_B = 5$ eV, (*a*) $\theta_A = 3°$, (*b*) $\theta_A = 5°$, (*c*) $\theta_A = 8°$.

The hydrogen ionisation data of Ehrhardt *et al.* (1985, 1986) are used in the next section for comparison with theory. They have been put on an absolute scale as described above. We have used their normalisation although we recognise the strength of the argument of Brauner *et al.* (1989) that it depends to some extent on the validity of the first Born approximation, which they have shown to be quite inadequate at the present energies in comparison with a much better calculation. The reader should recognise that the relative cross sections agree almost perfectly in shape with this calculation and consider whether to regard the calculation as a better way of normalising the experiments than the above methods, in spite of the agreement of the three somewhat independent determinations.

The relative experimental data of Lohmann *et al.* (1984), normalised to the second Born calculations of Byron *et al.* (1983), are included in the comparison in the next section. They essentially agree with the data of Ehrhardt *et al.*

To obtain a further clue to the normalisation question we have compared the DWBA for the total ionisation cross section to the experimental data of Shah *et al.* (1987), whose absolute determinations agree closely with their relative measurements normalised to the Born approximation at 500 eV. (Note that Brauner *et al.* find a significant but small departure of the three-body method from the Born approximation at 2000 eV for the differential cross sections considered.) At 150 eV the experimental and DWBA values (in $\pi a_0^2$) are respectively $0{\cdot}524\pm0{\cdot}006$ and $0{\cdot}63$. At 250 eV the corresponding values are $0{\cdot}389\pm0{\cdot}003$ and $0{\cdot}41$.

## 4. Comparison of Theory and Experiment

We have computed the differential cross section in the distorted-wave Born approximation (2), (3). It is represented in Figs 1–6 by solid curves. The pseudostate calculation of Curran and Walters (1987) is represented by long-dashed curves and the calculation of Brauner *et al.* (1989) by short-dashed curves. The solid circles represent the experimental data of Ehrhardt *et al.* (1985, 1986), and the open squares those of Lohmann *et al.* (1984).

The kinematic variables are defined as follows: $E_0$ is the incident kinetic energy; $E_A$, $\theta_A$ and $E_B$, $\theta_B$ are respectively the kinetic energy and polar angle (with respect to the incident direction) of the faster and slower electron. All three electron directions are coplanar. Units are eV and degrees.

We note first the essentially perfect shape agreement of the calculation of Brauner *et al.* with experiment and remind the reader to consider whether the experiments should be normalised to this calculation. Clearly the use of the three-body boundary condition is a major development in understanding ionisation.

The two methods that can at present be implemented in a scattering calculation are in reasonable semiquantitative agreement with each other and with experiment. We first consider the binary peaks at negative values of $\theta_B$. In general the DWBA produces somewhat larger values than the pseudostate method. Minor shape disagreements occur in the $E_B = 10$ and 14 eV cases for $E_0 = 250$ eV (Figs 2 and 3). In each case the DWBA is closer to the experimental peak. Both methods produce larger cross sections than the three-body method.

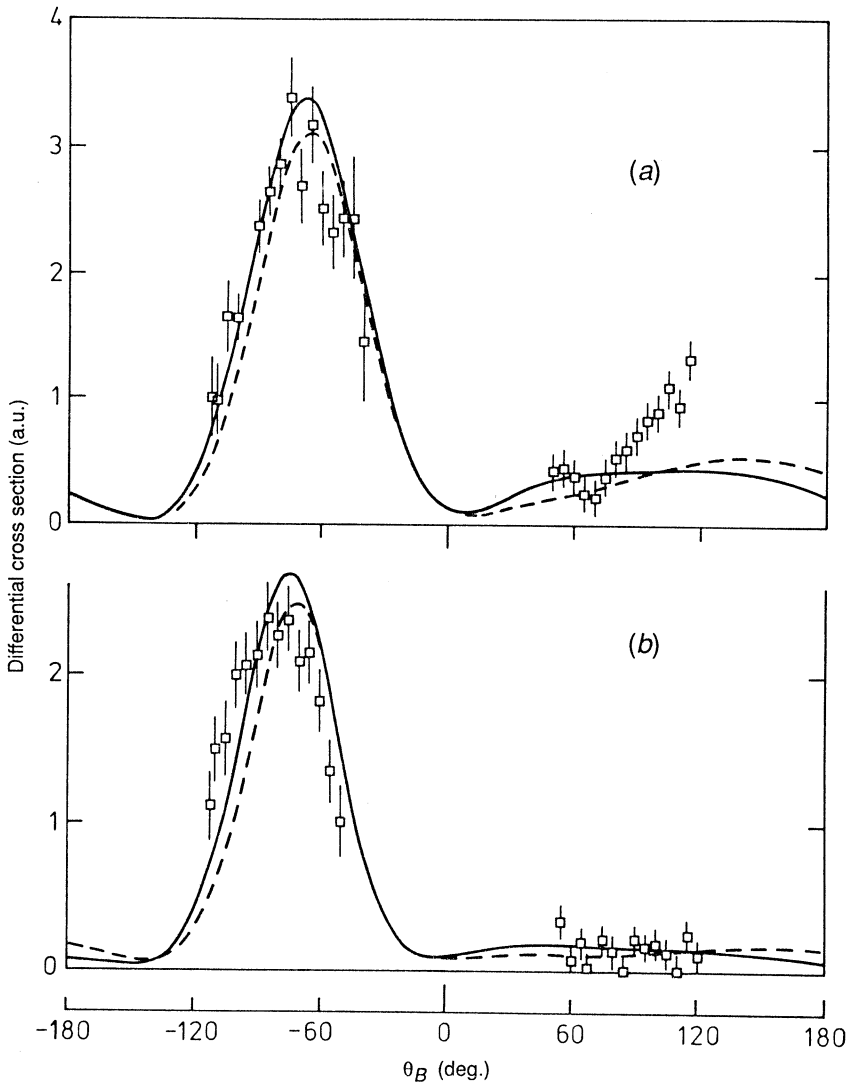


**Fig. 2.** As for Fig. 1 with $E_0 = 250$ eV, $E_B = 10$ eV, (*a*) $\theta_A = 5°$, (*b*) $\theta_A = 8°$.

For the smaller cross sections at positive values of $\theta_B$ there are more noticeable differences between various theories and with experiment. For $E_B = 5$ eV at $E_0 = 250$ and 150 eV there is very close agreement between the pseudostate and three-body calculations for the smallest values of $\theta_A$ (Figs 1*a* and 5*a*) and they both agree with the experimental trend. DWBA agrees roughly with the overall magnitude of the cross section but not at all in shape. For $E_0 = 250$ eV, $\theta_A = 5°$ and $E_B = 10$ and 14 eV (Figs 2*a* and 3*a*) the DWBA and pseudostate calculations agree qualitatively with each other but disagree

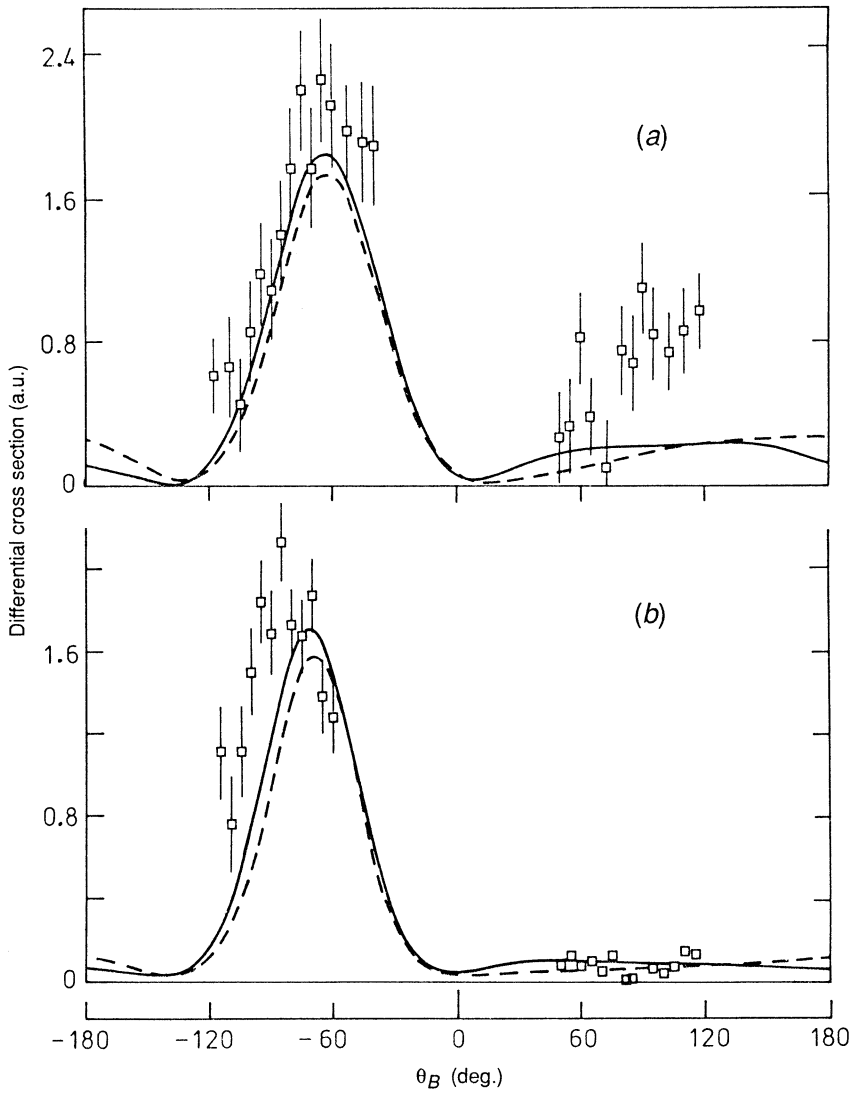


**Fig. 3.** As for Fig. 1 with $E_0 = 250$ eV, $E_B = 14$ eV, (*a*) $\theta_A = 5°$, (*b*) $\theta_A = 8°$.

markedly with experiment. For the largest values of $\theta_A$ in all cases cross sections for positive $\theta_B$ are quite small and qualitatively described by DWBA and the pseudostate calculation.

## 5. Conclusions

There is little to choose between the two methods for ionisation that can be implemented in a scattering calculation. These are the DWBA and the pseudostate method. Both agree at least semiquantitatively with relative

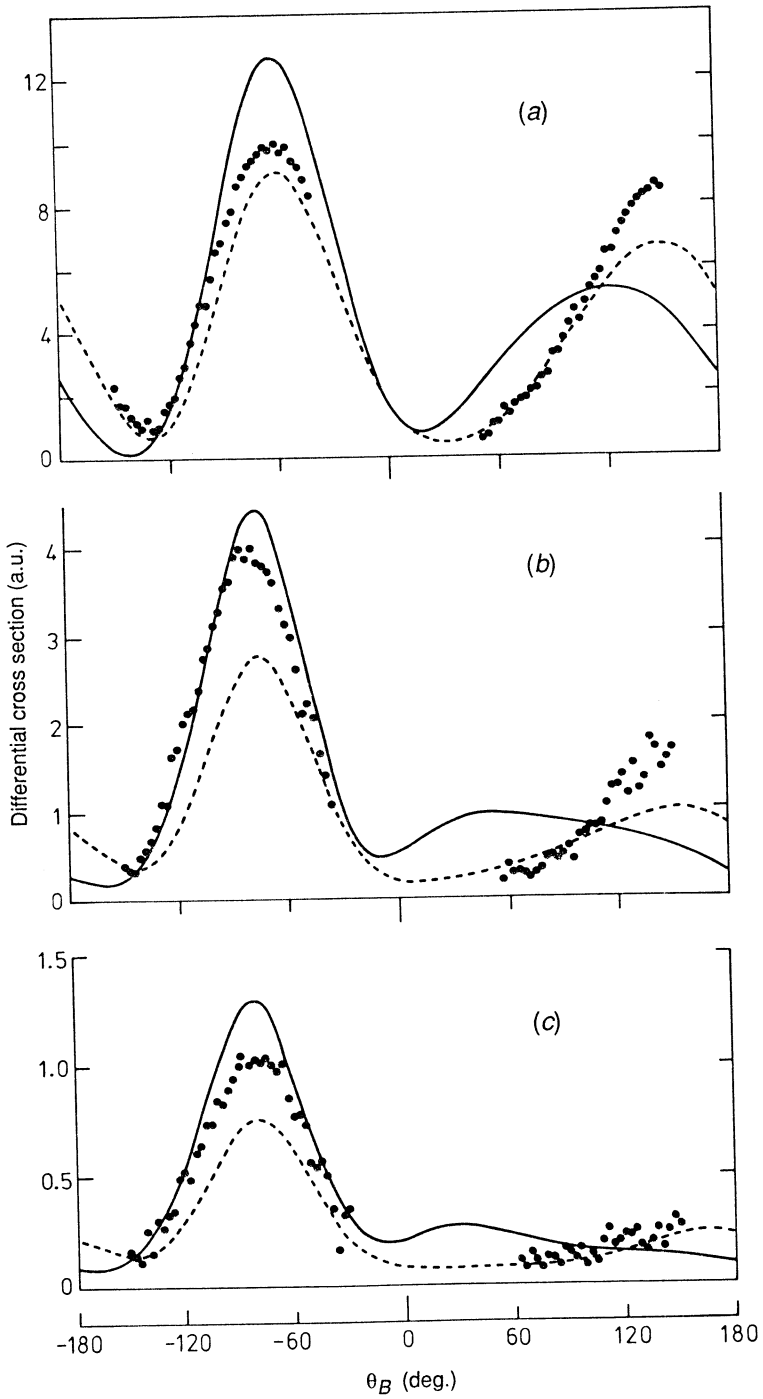


**Fig. 4.** As for Fig. 1 with $E_0 = 150$ eV, $E_B = 3$ eV, (*a*) $\theta_A = 4°$, (*b*) $\theta_A = 10°$, (*c*) $\theta_A = 16°$.

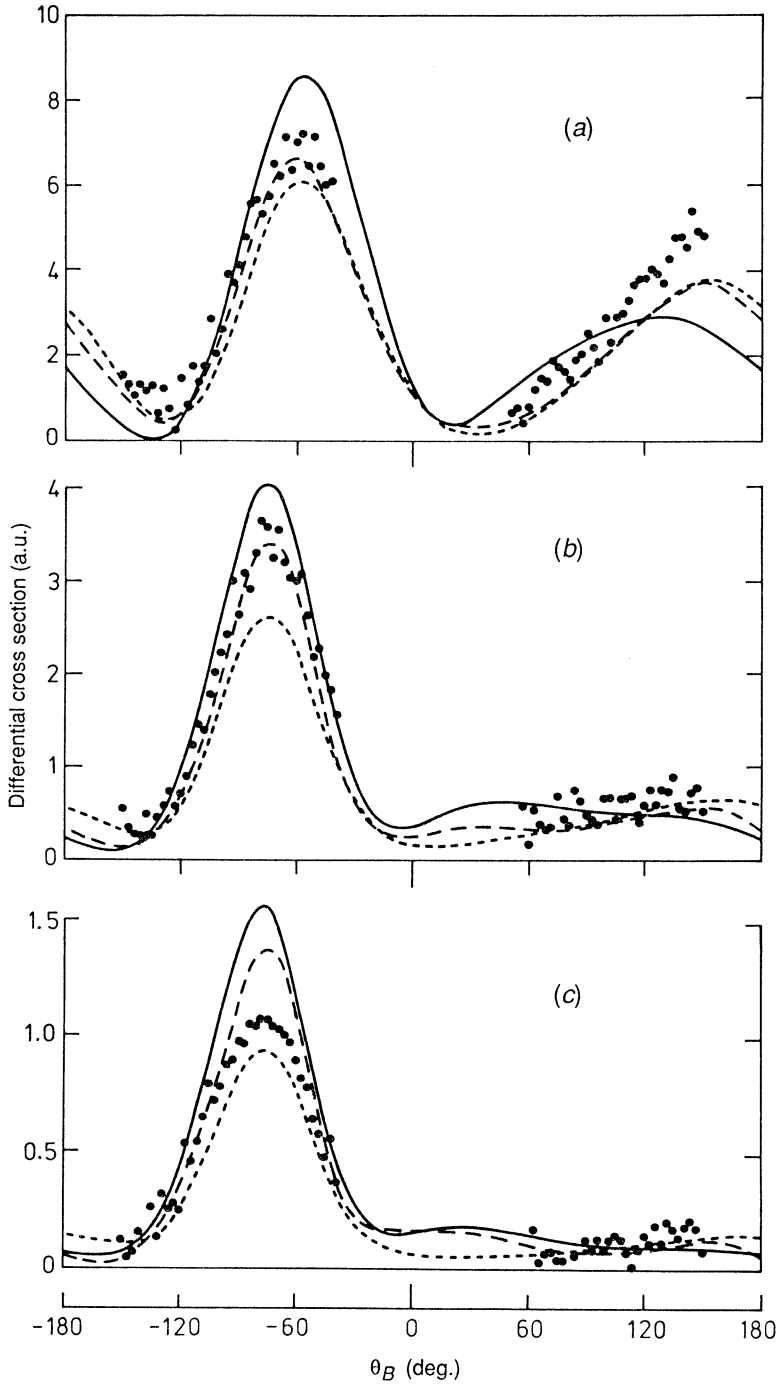


**Fig. 5.** As for Fig. 1 with $E_0 = 150$ eV, $E_B = 5$ eV, (*a*) $\theta_A = 4°$, (*b*) $\theta_A = 10°$, (*c*) $\theta_A = 16°$.

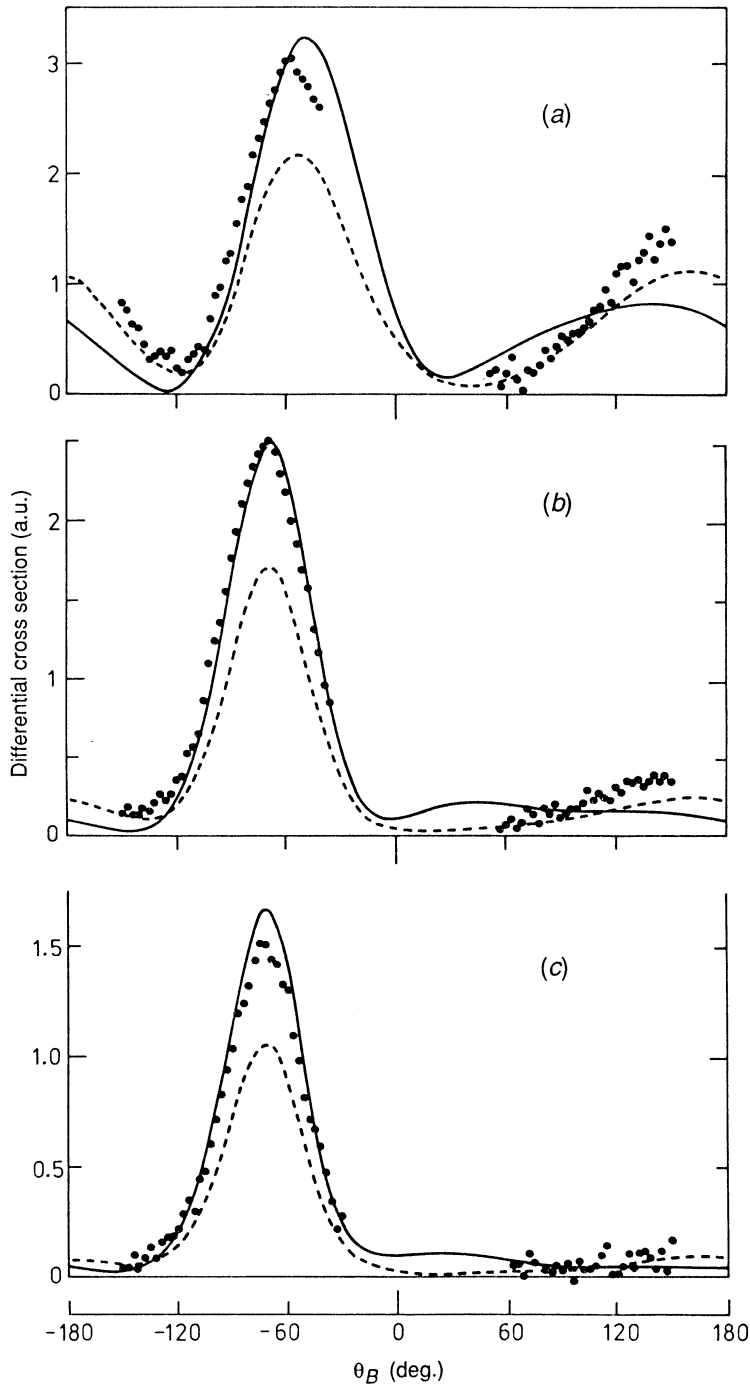


**Fig. 6.** As for Fig. 1 with $E_0 = 150$ eV, $E_B = 10$ eV, (*a*) $\theta_A = 4°$, (*b*) $\theta_A = 10°$, (*c*) $\theta_A = 16°$.

experimental cross sections normalised by methods that depend to some extent on the validity of the Born approximation. This is true particularly for the large cross sections in the binary peak. Here DWBA is somewhat larger and where there is slight shape disagreement DWBA is closer to experiment.

The implementation of the three-body boundary condition produces a dramatic shape improvement over the methods that involve essentially two-body physics. There is force in the argument of Brauner *et al.* (1989) that the Born approximation is so bad that it cannot be trusted to help in putting the relative experimental cross sections on an absolute scale. However at 150 and 250 eV the DWBA gives a total ionisation cross section in quite close agreement with experiment, suggesting that the absolute cross sections given by the three-body method are too low if we assume that the trend shown in the present differential cross sections remains for all of the kinematic space. In the present examples the three-body differential cross sections can be up to 30 percent lower than the DWBA cross sections.

It is clear that the implementation of the three-body boundary condition in the optical potential for the scattering problem would be a very promising direction for an ultimate understanding of scattering.

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