Electron impact ionisation of atomic hydrogen: experimental and theoretical (e, 2e) differential cross sections

E Weigold, C J Noble, S T Hood and I Fuss

Institute for Atomic Studies, School of Physical Sciences, The Flinders University of South Australia, Bedford Park, South Australia, 5042

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Abstract. Differential cross sections have been measured using coplanar kinematics for the electron impact ionisation of atomic hydrogen at incident energies of 100, 113.6, 250 and 413.6 eV for a variety of emitted electron energies and angles. The data are compared with differential cross sections calculated using: (i) the factorised distorted-wave half-off-shell impulse approximation (DWIA), (ii) the plane-wave impulse approximation (PWIA), and (iii) the plane-wave Born approximation with exchange (PWBE). The optical-model potential used to calculate the distorted waves is energy-dependent and has polarisation and exchange terms as well as an absorptive part. Various ways of treating the two outgoing electrons are examined in the DWIA. The use of different effective charges is investigated in the case when the two outgoing electrons are described as a product of Coulomb waves. Effective charges determined by asymptotic constraints give a poorer description of the data than simply using charges of unit magnitude. An approximation is also investigated in which the slower of the two outgoing electrons is treated as a Coulomb wave of unit charge and the faster is a distorted wave, the distorting potential being the ground-state optical-model potential. The results show that it is more important to know the wavefunctions in the region where all particles are interacting strongly, than to satisfy asymptotic constraints. The two plane-wave theories give completely inadequate fits to the data. The distorted-wave model gives a very much improved overall description of the data.

1. Introduction

A knowledge of electron impact ionisation and excitation cross sections for atomic systems is required for the understanding of many astrophysical and plasma phenomena. In particular a knowledge of ionisation cross sections is essential in the development of fusion research and technology. The most detailed information on the electron impact ionisation process is obtained in the determination of the (e, 2e) differential cross section, variously called the ‘triple’ (Ehrhardt et al 1971) or ‘five-fold’ (Schulz 1973) differential cross section. In general more than one final ion state can be excited, and the (e, 2e) cross section is then a ‘six-fold’ differential cross section.

The (e, 2e) cross section is a measure of the probability that an incident electron of energy $E_0$ will produce on collision two final-state electrons of energies $E_A$ and $E_B$ emitted into the differential elements of solid angle $\Omega_A$ and $\Omega_B$ respectively. ‘Double’ and ‘single’ differential and total cross sections involve integrations over some or all of the variables and generally smooth over the details of a particular theoretical calculation. Since the collision dynamics are completely specified in the (e, 2e) cross
section, it provides a fundamental testing ground for different theoretical approaches to
the ionisation problem.

Obviously the simplest ionisation problem is that of atomic hydrogen, involving only
two electrons and a proton. Whereas other ionisation problems are often complicated
by the use of different bound-state wavefunctions and potentials, these are known
exactly for atomic hydrogen, therefore permitting direct comparison of the approxima-
tions.

The Born approximation and its variants have been most widely used to calculate
ionisation cross sections. At sufficiently high energies it is generally believed that the
first Born approximation can be used to describe the direct ionisation process.
Unfortunately the range of validity of the Born approximation has not been
established. In any case, the energy at which the Born approximation becomes valid
depends on the system being studied and the kinematics of the outgoing electrons, and
at present it is not possible to specify over what energy or angular range the Born cross
section is accurate to within some given amount. It is therefore obviously necessary to
have a better theory than the first Born approximation, even at high energies but
especially in the range from threshold of ionisation to the 'high' energy regime.

Except for a recent preliminary report (Weigold et al 1977) on the ionisation of
atomic hydrogen, the simplest system studied in detail has been helium. Ehrhardt et al
(1969, 1971, 1972a, b) studied the cross section using asymmetric kinematics. Beaty et
al (1977, 1978) recently reported cross sections over similar kinematic regimes, but
also measured the cross section out of the plane. Hood et al (1973) measured the
non-coplanar symmetric differential cross sections \((E_A = E_B, \theta_A = \theta_B, \text{the azimuthal}
angle being the variable) at a number of energies and showed that this cross section was
directly proportional to the momentum distribution of ejected 1s electrons. McCarthy
et al (1974) and Dixon et al (1976) made detailed measurements of the symmetric
\((e, 2e)\) cross section to the \(n = 2\) state of the final He\(^+\) ion, and showed that this cross
section could only be explained if accurate correlated helium-target wavefunctions are
used.

The theoretical framework appropriate to the analysis of the symmetric geometry
experiments, in which the incident electron suffers a large momentum transfer, is the
half-off -shell impulse approximation (McCarthy and Weigold 1976). At sufficiently
high energies plane waves may be used to describe the incident and emitted electrons.
An eikonal approximation has also been used in the intermediate energy range to
describe the electron waves (Hood et al 1973, McCarthy and Weigold 1976).

Fuss et al (1978) recently used the full factorised distorted-wave half-off-shell
impulse approximation to calculate coplanar symmetric cross sections for helium at a
number of energies. They also used plane waves and 'eikonal' distorted waves in their
calculations. They found that the full distorted-wave calculations gave peaks in the
cross sections at too large an angle (relative to \(k_0\)), whereas the plane-wave theory gave
cross section maxima at angles significantly too far forward.

At high incident energies, small energy loss and small angle scattering of the incident
electron, the Born approximation may be more appropriate, although it has also been
applied to the prediction of symmetric cross sections (Neudachin et al 1968, Glassgold
and Talongo 1968). The asymmetric coplanar data of Ehrhardt and co-workers have
been compared with various Born approximation calculations. Jacobs (1974) and
Robb et al (1975) carried out plane-wave Born calculations in which the effects of using
well-correlated wavefunctions for the initial bound state and final ionic and low energy
free-electron state were explored. In both calculations the final free-target state was
described by a close-coupling wavefunction. The conclusion of Robb et al. (1975) was that the improvement of these wavefunctions did not guarantee a better agreement with the measured electron-electron angular correlations. The Born approximation, with the incident and fast outgoing electrons treated as plane waves, always predicts an azimuthal symmetry about the momentum transfer axis $K_{0A} = k_0 - k_A$, in disagreement with the data. The calculations of Jacobs (1974), Robb et al. (1975) and Burnett et al. (1976) indicate that it is not very useful to treat one aspect of the scattering problem (incident target and electron ejection) with high accuracy while treating in an elementary way the incident and fast outgoing electrons.

Of course, in the Born approximation only the direct scattering amplitude is considered, for which the scattered incident electron is the more energetic of the two ionising electrons. Ignored are the exchange process, for which the roles of the two electrons are interchanged, and the capture process, in which two 'target' electrons are excited to the continuum and the incident electron is captured into a bound state of the residual ion. The direct, exchange and capture processes are usually denoted by $f(k_A, k_B)$, $g(k_A, k_B)$ and $w(k_A, k_B)$ (Rudge 1968) where convention has $k_A \geq k_B$.

Phillips and McDowell (1973) showed the capture process to be unimportant in helium, except in regions of energy and angle where the exchange cross section is negligible. They represented the incident and the faster of the two outgoing waves by plane waves. The capture process is of course completely absent in the ionisation of hydrogen.

Schulz (1973) used a product of Coulomb wavefunctions in the final state, to calculate $(e, 2e)$ cross sections for helium and hydrogen. In the case of helium he used a simplified ground-state wavefunction. In addition to the direct amplitude, he determined the exchange amplitude (and, for helium, also the capture amplitude). Schulz investigated the effect of various nuclear screening parameters on the ionisation cross section, within the context of the Born model.

Geltman and Hidalgo (1974) and Geltman (1974) used the Coulomb-projected Born approximation, including exchange, to calculate similar cross sections for hydrogen and for helium. The Born calculations of Schulz (1973), Geltman and Hidalgo (1974) and Weigold et al. (1977) are the only ones which have been carried out for the case of atomic hydrogen as a target. In the Coulomb-projected Born approximation (CPB) both outgoing electrons are presented as continuum states of the hydrogen atom (Coulomb functions). It has the advantage that it includes the exchange in a more physically reasonable way than can be done in the plane-wave approximation, since the CPBE approximation satisfies the relation

$$g(k_B, k_A) = f(k_A, k_B)$$

required by the indistinguishability of electrons. Since the CPB direct amplitude is a function of the three vectors $k_A$, $k_B$, and $K_{0A}$, the axial symmetry about the momentum transfer vector $K_{0A}$ is no longer present. This symmetry disappears even in the PWBA when exchange is included by putting $g(k_B, k_A) \equiv f(k_A, k_B)$.

Madison et al. (1977) reported the results of a distorted-wave first Born approximation calculation for the ionisation of helium. It is closely related to the zero-order many-body theory calculation of Baluja and Taylor (1976). Madison et al. (1977) chose the same distorting potential in both incident and exit channels. It is simply the interaction between the target nucleus and the incident electron together with the spherical average of the static interaction between the incident electron and the atomic
electrons in the ground state. The ground state is described by a Hartree–Fock wavefunction.

Baluja and Taylor also calculate both distorted waves in the field of the ground state, using the static-exchange approximation. Using the same neutral potential for the ingoing and fast emerging electron (one of the two-time models of Baluja and Taylor) gives amplitudes which are not time-reversal invariant. The usual argument presented for this non-physical two-time model (e.g. Baluja and Taylor) is that the ‘passage time’ of the projectile is much smaller than the ‘excitation time’. The wavefunction of the slow continuum electron is then an orbital with Coulomb boundary conditions and the static (exchange) potential of the He\(^+\) ion.

The distorted-wave Born calculations, which include the exchange as well as the direct amplitudes, give in general a better agreement with the asymmetric data of Ehrhardt et al. (1969, 1972a, b) than obtained with the plane-wave or Coulomb-projected Born approximations.

In the present work we present some experimental and theoretical results for the electron impact ionisation of atomic hydrogen. In §2 we give an outline of the experimental technique and in §3 the theories. In §4 we compare the results with various calculations. These include the plane-wave Born, plane-wave half-off-shell impulse approximation and the distorted-wave impulse approximation. In particular, various proposals for treating the outgoing electrons are considered in detail. These include an investigation of the effective-charge method of Rudge (1968) and Peterkop (1962) as well as the somewhat non-physical two-time model in which the fast electron ‘sees’ an effective neutral atom in both the initial and final channels.

2. Experiment

Measurement of the \((e, 2e)\) differential cross section involves the determination of the momenta of the incident \((k_0)\) and two emitted electrons \((k_A\) and \(k_B\)). The geometry is defined relative to the incident direction \((k_0)\), the two final continuum electrons of energy \(E_A\) and \(E_B\) being emitted at angles \((\theta_A, \phi_A)\) and \((\theta_B, \phi_B)\) respectively. The present experiments were carried out in coplanar geometry so that \(\phi_A - \phi_B = 0\) or \(\pi\). When the emitted electron energies are not equal we follow the convention of labelling the faster electron by the subscript \(A\) and the slower by \(B\). Then electron \(A\) is usually known as the ‘scattered’ electron and electron \(B\) as the ‘ejected’ electron, although it must be remembered that the two are of course indistinguishable.

The energy and momentum conservation equations are

\[ \epsilon = E_0 - E_A - E_B \tag{1} \]

and

\[ q = k_0 - k_A - k_B = K_{0A} - k_B \tag{2} \]

where \(q\) is the recoil momentum of the ion, and \(K_{0A} = k_0 - k_A\) the conventional momentum transfer. The separation energy of the electron is \(\epsilon\) (for simplicity the ion recoil energy is ignored).

The coplanar electron coincidence spectrometer is a modified version of the one described in detail by McCarthy and Weigold (1976) and by Fuss et al. (1978) and only a brief description need be given here. Figure 1 shows the apparatus schematically. It is
mounted on the bottom plate of an aluminium and stainless-steel bell-jar vacuum chamber. A 10 cm oil diffusion pump and a liquid nitrogen trap pump the chamber through a port in this plate.

Two cylindrical-mirror electron energy analysers and their associated collimators and retarding lenses are used to determine the energies and polar angles of the two emitted electrons. The analysers are mounted on two concentric turntables, which can be rotated independently in either direction by stepping motors. The turntables are maintained concentric to a high degree of precision by bearings mounted below and between the tables. The stepping motors are controlled by a PDP-11 computer and, with the aid of suitable gears, can set the angular positions of the analysers to better than 0·2°.

The electron gun is of conventional design and employs a thoriated tungsten wire filament. It is mounted inside a stainless-steel jacket, and typical operating currents are in the range of 0·1−1·0×10⁻⁶ A with an energy half-width of about 0·3 eV. The unscattered beam is collected in a deep Faraday cup which is retractable to allow measurements at small angles. The cup consists of an inner cylinder of diameter 0·4 cm and an outer cylinder of 1·0 cm diameter, the latter measuring the ‘spray’ current. This is always negligible, since collimators in front of the gun limit the maximum angular divergence of the beam to 1°. Helmholtz coils and mu-metal shielding reduce stray magnetic fields to less than 10 mG within the experimental region. Care is taken to use non-magnetic materials in the construction of the apparatus.
Collimating apertures placed before the retarding lens define the angular field of view of the electron detectors. The three element lenses form an image on the entrance apertures, which are on the axes of the concentric cylindrical-mirror analysers. After traversing the cylindrical-mirror analysers the electrons are detected by channel electron multipliers (CEM).

The interaction region is defined by the intersection of the electron and atomic-hydrogen beams. With the present source of atomic hydrogen (see Hood et al 1978 for details), 90% of the density integrated along the electron beam occurs in a length significantly smaller than 8 mm, the electron beam being less than 1.5 mm in diameter. If the angular settings of both detectors are changed in a measurement, it is necessary to ensure that both view the entire collision region. Most measurements were, however, carried out with detector A (i.e. fast-electron detector) at a fixed angular setting. It is then only necessary to ensure that the field of view of the moving analyser is larger than the collision region, now defined by the intersection of the electron and atomic-hydrogen beams and the viewing angle of the stationary detector. In these measurements it is important to keep the viewing angle of detector A small, especially for small $\theta_A$.

Details of the DC discharge tube atomic-hydrogen source (Wood's tube) are given in Hood et al (1978). The tube, shown schematically in figure 1, has a total length of 1.7 m. The hydrogen gas (sometimes containing up to 2% of water vapour) is leaked into the discharge tube near the cathode through a capillary tube. The cathode region and the discharge tube inside the vacuum system are water cooled. The tube is constructed from pyrex except for the cathode region and the exit tube leading to the scattering region. These are made of silica. The exit tube is approximately midway between the hollow aluminium electrodes. Hydrogen effuses vertically down through a 1 mm hole in the centre of the silica endplate of the exit tube, through a channel in a 2 mm thick PTFE support, a 0.5 mm diameter aperture in a tantalum plate and a 0.8 mm diameter hole in a brass support plate, all coaxial with the turntables carrying the electron detectors. The centre of the electron beam is typically 2 mm below the brass plate. Support is given by three adjustable nuts on brass studs mounted on a hollow brass pillar. The whole region is grounded and coated with colloidal graphite. Care is taken to screen against all stray electric fields.

Typically the discharge runs at a current of 30-50 mA with a potential drop from the anode to the grounded cathode of about 4 kV. The dissociation is generally of the order of 80% (see Hood et al 1978 for details) and the coincidence separation-energy spectra clearly show a peak at $\epsilon = 13.6$ eV and a much smaller peak at $\epsilon = 15.9$ eV, due to H and $\text{H}_2$ respectively (Weigold et al 1977). Transitions in $\text{H}_2(e, 2e)\text{H}_2^+$ from excited vibrational states of $\text{H}_2$ can interfere with the $\text{H}(e, 2e)\text{H}^+$ signal. In particular the transitions $\nu'' = 4 \rightarrow \nu' = 0$ has $\epsilon = 13.5$ eV and $\nu'' = 3 \rightarrow \nu' = 0$ has $\epsilon = 14.0$ eV. However the production in the discharge of the $\nu'' = 3$ and 4 states is negligible, the density of these states in the interaction region being at least two orders of magnitude less than that of atomic hydrogen (Hood et al 1978). The density of atomic hydrogen in the target region is approximately $2 \times 10^{18} \text{ m}^{-3}$. The background gas density is two orders of magnitude less. With the discharge off, only the peak at 15.9 eV is evident, with no counts at 13.6 eV. The energy resolution is approximately 1.0 eV FWHM.

Since only a tiny fraction of the counts in each channel is due to a pair of electrons originating from the same ionising event, coincidence techniques must be used. The signal processing and fast timing electronics are outlined in figure 2. Pulses from the channel electron multipliers (CEM) at the exit apertures of the two cylindrical-mirror...
analysers (CMA) are amplified, and timing signals from zero-crossing discriminators are fed to the start and stop inputs of a time-to-amplitude converter (TAC). The TAC output has a flat background due to the arrival of pulses from uncorrelated electrons, as well as a peak centred around a particular pulse height due to events with a given time correlation. Two single-channel analysers (SCA) view respectively the correlated or coincidence region (C) and the flat background region (B). The width of window B is 15 times as large as that of C in order to reduce the error in background subtraction (McCarthy and Weigold 1976), the width of window C being 9 ns. The outputs of windows C and B are monitored by CAMAC scalers, the PDP-11 mini-computer keeping track of the true signal (C−B/15) as well as the statistical error. The TAC output and the SCA windows are also monitored by the computer-based pulse-height analyser (MCA).

The coincidence count rate is first measured as a function of the incident energy for fixed angles $\theta_A$ and $\theta_B$ and fixed energies $E_A$ and $E_B$. Next the angular correlation is measured for the atomic-hydrogen transition. The computer sets the corresponding energies and angles. At each energy and angle the computer records the counts in the coincidence and background scalers after being triggered by the preset scaler, calculates the number of real coincidences (after taking account of the relative channel widths), calculates the statistical error, sets new angles (or energies) for the analysers, and then restarts the scalers. The time spent at each energy and angle is quite brief, and the effects of long term fluctuations in intensities are minimised by scanning through the

Figure 2. Schematic diagram of the (e, 2e) spectrometer and associated fast timing and data processing electronics. Voltage supplies for the channel electron multipliers, and cylindrical-mirror analysers, retarding lenses, electron gun etc are not shown.
angular range many times, usually of the order of 100 scans per experimental run. In each angular scan each combination of angles is covered and recorded separately on four occasions, in order to check the internal consistency of the data at each angular setting.

In nearly all of the data reported here only the angle $\theta_B$ of the slower (or ejected) electron is varied for a fixed angle $\theta_A$. Several angular correlations at different $\theta_A$ are then put on the same relative scale by fixing $\theta_B$ and varying $\theta_A$. In both cases the moving analyser views at all angles the whole interaction region defined by the overlap of the view of the fixed analyser and the atom and electron beams. The preset scaler is triggered by pulses from the fixed detector, in order to normalise the data of the same integrated number of collisions. In the experiment for which $\theta_A$ and $\theta_B$ were both varied (and kept equal), the preset scaler is triggered by pulses from a voltage-to-frequency converter which measures either the electron current or the average atomic-beam intensities. These both have a long term stability of a few percent.

The computer keeps a cumulative result of the counts for each angle and energy and displays it, the error, scan number, energy, angle, etc at each setting of the analysers. The data are printed out on demand or at regular intervals after a given number of scans to give a further check on the consistency of the data.

Each angular correlation involves a counting period of the order of 24 hours, and sometimes up to 76 hours.

3. Theory

3.1. Distorted-wave impulse approximation

In the half-off-shell distorted-wave impulse approximation (McCarthy and Weigold 1976, Hood et al. 1973), the absolute magnitude of the (e, 2e) differential cross section is given by

$$\frac{d^5\sigma}{d\Omega_A d\Omega_B dE_A} = (2\pi)^4 \frac{k_A k_B}{k_0} \sum_{av} |M(k_A, k_B)|^2$$

where $\Sigma_{av}$ denotes the usual procedure of summing over the final states and averaging over the initial states, and symmetric normalisation has been adopted (Weigold and McCarthy 1978).

The distorted-wave amplitude is given by

$$M(k_A, k_B) = \langle \chi_A^{(-)}(k_A) \chi_B^{(-)}(k_B) | T_M(p^2) | f | g \rangle \chi_0^{(+)}(k_0)$$

where $T_M$ is the antisymmetrised two-electron (Mott-scattering) $T$ matrix, $(f|g)$ is the overlap function of the target state $|g\rangle$ and final ion state $|f\rangle$, and $\chi^{(+/-)}$ are optical-model wavefunctions describing elastic scattering in the appropriate two-body subsystems.

In order to make the calculation tractable it is necessary to make the factorisation approximation (McCarthy and Weigold 1976). This approximation is exact in the eikonal or plane-wave limits. The cross section then becomes for hydrogen

$$\frac{d^3\sigma}{dE_A d\Omega_A d\Omega_B} = \frac{(2\pi)^4 k_A k_B}{k_0} |T_M|^2 \frac{1}{(2\pi)^3} |\langle \chi_A^{(-)}(k_A) \chi_B^{(-)}(k_B) | \psi_{1s}(r) \chi_0^{(+)}(k_0) \rangle|^2$$
where $|T_M|^2$, the half-off-shell Mott-scattering cross section, is given by

$$|T|^2 = \left| \frac{1}{2}(k_A - k_B) / t_c (p^2)^{1/2} (k_0 + p) \right|^2$$

$$= \frac{1}{4\pi^4} \frac{2\pi \eta}{(2\pi)^{3/2}} \left[ \frac{1}{|k - k'|^2} + \frac{1}{|k + k'|^2} - \frac{1}{|k - k'|^2 |k + k'|^2} \cos \left( \eta \ln \left( \frac{|k + k'|}{|k - k'|} \right) \right) \right]$$

and

$$\eta = 1/2k', \quad k' = \frac{1}{2}(k_A - k_B), \quad k = \frac{1}{2}(k_0 + q), \quad p^2 = k^2.$$  (7)

Here $q = k_0 - k_A - k_B$ is the ion recoil momentum. In the plane-wave limit $q$ is the momentum of the target electron, and the cross section reduces to

$$\frac{d^2\sigma}{dE_A d\Omega_A d\Omega_B} = 4\pi^2 \frac{k_A k_B}{k_0} |T|^2 R_{1s}(q)$$

where

$$R_{1s}(q) = \left( \frac{2}{\pi} \right)^{1/2} \int_0^\infty r^2 d\rho j_0(qr) R_{1s}(r)$$

is the radial momentum distribution of the target hydrogen electron.

In order to evaluate the second factor in equation (5) the distorted waves $\chi_A, \chi_B$, and $\chi_0$ must be calculated. They are computed directly from optical-model potentials by solving the distorted-wave equations for elastic scattering in the relevant channel in partial-wave form and performing the radial integral and partial-wave sums explicitly.

### 3.1.1. Optical-model potentials

In the present work we have used the optical model of Vanderpoorten (1975) to calculate the wavefunction of the incident electron. This local central potential is energy-dependent and of the form

$$V(r) = V^{(1)}(r) + V^{(2)}(r) + V_E(r).$$

The first term is the static potential, which corresponds to the first-order term in a multiple-scattering expansion of the interaction and is given by $V^{(1)}(r) = \langle 0 | V | 0 \rangle$, where $|0\rangle$ is the hydrogen ground-state wavefunction and $V$ is the sum of the electron–electron and electron–proton Coulomb potentials.

The potential $V^{(2)}(r)$ is a central approximation of the exact eikonal second-order potential. The large $r$ behaviour of the potential is imposed by having the real part of the potential, which exhibits $r^{-4}$ behaviour, give the dipole polarisation potential. Thus

$$\text{Re} \ V^{(2)}(r) \sim -\alpha/2r^4.$$  (11)

The imaginary part of the second-order potential describes the loss of electrons from the elastic channel. The variation of $\text{Im} \ V^{(2)}(r)$ for large $r$ is $r^{-6}$.

The equivalent exchange potential $V_E(r)$ is obtained by localising the exchange potential appearing in the appropriate continuum Hartree–Fock equations. The resulting triplet and singlet potentials may be written (Vanderpoorten 1975)

$$V^\pm_E(r) = \frac{1}{2}(E - V^{(1)}(r) - [(E - V^{(1)}(r))^2 + 32|\psi_{1s}(r)|^2]^{1/2}).$$  (12)
The radial Schrödinger equation is then solved exactly for this optical-model potential by the partial-wave method. This gives the (complex) phaseshifts of the electron waves $\chi^n(k)$ at the corresponding incident energy.

The differential cross sections for electron–hydrogen elastic scattering computed with this potential (Vanderpoorten 1975) are in excellent agreement with those calculated by Winters et al (1974), who employed the full non-local second-order potential and exchange kernels. The worst observed disagreement is of the order of 10% and occurs at the most forward angles for the low energy of 50 eV. At intermediate energies the agreement is also good with the experimental data of Lloyd et al (1974), Williams (1975) and Van Wingerden et al (1977).

Madison et al (1977) in their distorted-wave calculation of the (e, 2e) cross section used only the static potential $V^{(1)}(r)$ to calculate their distorted waves, whereas Baluja and Taylor (1976) used the static-exchange approximation. Neither allowed for the long-range polarisation effects or absorption of the electron waves due to the open channels.

### 3.1.2. Exit-channel distorted waves

In the three-body final state the particles all interact via the long-range Coulomb force. Various proposals have been made to treat the difficult problem of the two continuum electrons. These range from time arguments (e.g. Baluja and Taylor 1976) to the use of effective charges (Rudge 1968). None of the proposals take into account the simultaneous correlation of all three particles at all distances from each other.

The asymptotic Coulomb interactions between all three bodies in the final state can be dealt with by the method reviewed by Rudge (1968). It was used by Fuss et al (1978) in their factorised distorted-wave impulse approximation calculations and by Schulz (1973) in his Born calculations. Effective charges $Z_A$, $Z_B$ for the two final electrons of momenta $k_A$ and $k_B$ are chosen so as to remove the logarithmic singularity in the phase of the (e, 2e) amplitude. In atomic units this is

$$\lim_{\rho \to \infty} \exp[i(1/k_A + 1/k_B - 1/|k_A - k_B| + Z_A/k_A + Z_B/k_B) \ln 2X]\, (13)$$

where

$$X^2 = k_A^2 + k_B^2.\, (14)$$

The condition determining the effective charges is therefore

$$\frac{1 + Z_A}{k_A} + \frac{1 + Z_B}{k_B} = \frac{1}{|k_A - k_B|}.\, (15)$$

The same result is obtained classically by requiring the energy of the two effective charges interacting with the ion, but not with each other, to be the same as the energy of the system of two electrons and the ion with Coulomb forces between all pairs.

In the case of hydrogen, with a proton and two free electrons in the final state, the distorted waves $\chi^{(c)}_{A(B)}$ are simply Coulomb waves with the effective charges $Z_A$ and $Z_B$. The differential cross section is then proportional to (Fuss et al 1978):

$$\sigma = |f(k_A, k_B)|^2 + |f(k_B, k_A)|^2 - \text{Re}[f(k_A, k_B)^* f(k_B, k_A)] \, (16)$$

where

$$f(k_A, k_B) = -(2\pi)^{-5/2} M'(k_A, k_B) e^{i\lambda}$$
and

$$\Delta(k_A, k_B) = 2[(Z_A/k_A) \ln(k_A/X) + (Z_B/k_B) \ln(k_B/X)].$$

The matrix element $M'$ is equivalent to the direct term of (4).

The asymptotic condition (15) does not determine $Z_A$ and $Z_B$ uniquely, and a further constraint is required. By imposing the additional condition that the field strength at the nucleus be changed only minimally by the introduction of the effective charges, they are given by

$$Z_A = -1 + \frac{k_A[k_A \cdot (k_A - k_B)]}{|k_A - k_B|^3} \quad Z_B = -1 + \frac{k_B[k_B \cdot (k_B - k_A)]}{|k_B - k_A|^3}.$$ (17)

This approximation, which is the approximation (A6) of Schulz (1973), gives effective charges which differ at every angle. The computation must therefore be done completely at each angle and energy. The full calculation (DWIA-2) was therefore only performed in some special cases and compared with a simplified model (DWIA-3) taking average effective charges. These 'average' values were the values of $Z_A$ and $Z_B$ obtained from (17) for the value of $k_B$ corresponding to the observed maximum in the differential cross section.

In order to simplify the calculations, the standard approximation (DWIA-1) adopted was to choose

$$Z_A = Z_B = -1.$$ (18)

This approximation assumes that both electrons see the full charge of the proton, both outgoing waves being Coulomb waves of unit charge. This violates the asymptotic condition (15) in general, although it satisfies it in the limit $|k_A - k_B| \gg 1$. On the other hand the asymptotic effective charges may lead to the wrong description when the particles are close to each other and interacting strongly.

Since the effective charges appear in the wavefunction in the asymptotic region in the combination $Z_{\text{eff}}/k$, the influence of the effective charge $Z_B$ of the slower electron will obviously be very much greater than that of $Z_A$. Therefore one further approximation was investigated. As the faster outgoing electron leaves the collision region it feels the influence of the slower electron and proton diminish rapidly. The slower electron, which remains relatively close to the proton, essentially screens the proton. Complete screening gives $Z_A = 0$, the faster electron 'seeing' an effectively neutral atom, which is however in a continuum orbital. However $Z_A = 0$ would give a plane wave for $\chi''$ whereas the faster incoming electron which also 'sees' a proton–electron system (but bound in this case) is a fully distorted wave. To be consistent it is necessary to treat the fast outgoing electron in this approximation in an analogous way to the incoming electron. The optical-model potential for the incident electron is calculated for a ground-state hydrogen-atom target system. Obviously time-reversal invariance requires that the optical potential for $\chi_A(k_A)$ be calculated at energy $E_A$ and for a 'target' system consisting of a proton and a continuum electron (of energy $E_B$). In order to simplify this formidable task, we have calculated the outgoing distorted wave using the same form (10) for the optical potential as for the incoming electron.

This approximation (DWIA-4) is similar to the two-time approximation of Baluja and Taylor (1976) and the approximation of Madison et al (1977). The potentials used by these workers were, however, energy independent, and did not allow for polarisation effects and absorption. The present potential is dependent on the different energies $E_0$.
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and $E_A$ of the incident and fast electron, and so in the present calculation the potentials are different in the incident and exit channels. Further, if this model is valid $Z_B$ must be close to $-1$ (see equation (17)) since this model assumes $k_A >> k_B$. In order to simplify the calculations we have therefore chosen $Z_B = -1$ at all angles, i.e. the slow outgoing electron is a Coulomb wave. This approximation places stress on knowledge of the wavefunction near the target where overlap with the bound-state function is large.

3.2. The plane-wave impulse approximation (PWIA)

Calculations were also carried out in the plane-wave impulse approximation given by (8), which also obviously includes the effects of exchange. This cross section is given by the product of two factors: the electron momentum distribution $R_A(q)$ (equation (9)) and the half-off-shell Mott-scattering cross section (equation (6)). The former has a maximum at $q = \frac{k_0 - k_A - k_B}{2}$, whereas the Mott-scattering cross section increases as $\theta_{BA} = \theta_A + \theta_B$ decreases.

3.3. The plane-wave Born approximation with exchange (PWBE)

In order to compare the half-off-shell impulse approximation with the Born approximation, which continues to provide a popular reference for ionisation calculations, calculations were also performed for the plane-wave Born approximation with exchange included. In this approximation, in which all electrons are described by plane waves as in PWIA, the direct scattering amplitude is given by

$$f(k_A, k_B)_{PWBA} = \frac{8\sqrt{2}}{(2\pi)^3} \frac{(1 + q^2)^2 - (1 + k_B^2)^2}{|k_0 - k_A|^2}$$

(19)

and the exchange amplitude is simply given by

$$g(k_A, k_B) = f(k_B, k_A).$$

(20)

The cross section is given by

$$\frac{d^3\sigma}{d\Omega_A d\Omega_B dE_A} = (2\pi)^4 \frac{k_A k_B}{k_0^2} (f^2 + g^2 - fg).$$

(21)

The common factor $1/|k_0 - k_A|^2$ is just the Rutherford amplitude. The expression shows that the momentum transfer is shared by the ion (with recoil momentum $q$) and the slow electron (with momentum $k_B$). Examination of (19) also shows that the PWBA direct amplitude has azimuthal symmetry about the recoil $q = 0$ axis, unlike the PWIA.

The first term in (19) gives rise to what is commonly called the binary-encounter peak at $q = 0$, whereas the second term (which changes the sign of $f$ for $q > k_B$) may give rise to a 'recoil' peak. The two peaks in $|f|^2$ are then necessarily separated by zeros.

4. Results and discussion

The measured angular correlations are summarised in table 1. Since absolute cross sections were not obtained, the cross sections are all normalised to a maximum of 100 in any set of independent measurements. The numbers in parentheses give the errors in the last significant figure. At the incident energies of 413.6, 250 and 113.6 eV the
differential cross sections have also been measured as a function of $\theta_A$ as well as $\theta_B$. This means that at these energies only one arbitrary normalisation factor is required, and the percentage errors in the normalisation of the various differential cross sections at different $\theta_A$ are indicated in table 1 by $\sigma_N$. This error has not been included in the errors given in the parentheses. At $E_0 = 100$ eV the measurements at different $\theta_A$ are all independent and have all been separately normalised to a maximum of 100 in any individual angular correlation.

The measured differential cross sections are compared with various theoretical calculations in figures 3–8. Three different approximations are investigated at all energies and angles. These are the plane-wave Born approximation with exchange (PWBE) discussed in § 3.3, the plane-wave half-off-shell impulse approximation, which includes exchange and is discussed in § 3.2 (PWIA), and the distorted-wave half-off-shell impulse approximation with full effective charges $Z_A = Z_B = -1$ in the exit channel. This latter is designated the DWIA-1 model (see § 3.1).

Figure 3 shows the data at $E_0 = 413.6$ eV, $E_A = E_B = 200$ eV, $\phi_A - \phi_B = \pi$. The data is normalised to the DWIA-1 cross section at $\theta_A = 40^\circ$, $\theta_B = 45^\circ$. For ease of comparison the calculated cross sections based on the other approximations are normalised to give the same peak height in the $\theta_A = 40^\circ$ angular correlation. The multiplication factors are also shown in the figure, the plane-wave cross sections being

<table>
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<th>( \theta_A ) (deg)</th>
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<td>15</td>
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<tr>
<td>113.6</td>
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<tr>
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<td>20</td>
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<td>80(23) 85(24) 90(25) 95(26) 100(27) 105(28) 110(29) 115(30)</td>
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</tbody>
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Table 1. Summary of the measured H(e, 2e)H$^+$ differential cross sections. The maximum value in each independent set of measurements has been normalised to the value of 100. The figures in brackets give one standard deviation error for the corresponding point in the cross section. The percentage error in the normalisation of data at different $\theta_A$ is given by $\sigma_N$. $\phi_A - \phi_B = \pi$ except for the case $\theta_A = 20^\circ$ indicated by + for which $\phi_A - \phi_B = 0$. 
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considerably larger than the distorted-wave cross sections. The DWIA-2 approximation is also investigated at this energy. In this model the effective charges on the outgoing distorted waves are determined by the asymptotic condition of Rudge (equation (15)). In this particular case we can set $Z_A = Z_B$ (since $k_A = k_B$), and equation (15) is sufficient to fix both $Z_A$ and $Z_B$, it being unnecessary to invoke any further constraint. $Z_A$ and $Z_B$ range from $-0.5$ at $\theta_A = \theta_B = 30^\circ$ to $-0.71$ at $\theta_A = \theta_B = 60^\circ$. As expected from the asymptotic considerations, at large relative angles of emission, screening of the proton charge becomes relatively less important. However, figure 3 shows quite clearly that the DWIA-1 model with $Z_A = Z_B = -1$ gives a much better description of the data at the smaller angles $\theta_{AB}$ ($= \theta_A + \theta_B$ for $\phi_A - \phi_B = \pi$), whereas the DWIA-2 approximation provides a somewhat better description at ‘backward’ angles ($\theta_{AB} > 90^\circ$). The small (or forward angles in the CM system) correspond to lower momentum transfer $K_{0A} = |k_0 - k_A| \leq 3a_0^{-1}$, whereas at larger angles $K_{0A} \geq 4a_0^{-1}$. Since the DWIA-1 model does better at lower $K_{0A}$ and the DWIA-2 model does significantly better at higher $K_{0A}$, the data imply that the effective charges should decrease slightly with increasing $K_{0A}$, instead of the opposite trend required by the asymptotic condition.

Both plane-wave approximations (PWBE, PWIA) predict cross sections in very serious disagreement with the data even at the relatively high incident and exit energies.
involved in this case. The plane-wave cross sections are much too large at small \( \theta_A \) and \( \theta_B \), and much too small at large \( \theta_A \) and \( \theta_B \). The PWBE cross sections are generally a factor of 2 or so higher than the corresponding PWIA cross sections. At angles \( \theta_B \gtrsim 45^\circ \) the PWIA and PWBE curves are almost indistinguishable with the normalisation used, and for simplicity only the PWIA curve is shown at these angles. In the figure the crosses, open circles, filled circles and triangles indicate the cross sections for \( \theta_A = \theta_B, \theta_A = 30^\circ, 40^\circ \) and \( 50^\circ \) respectively. The calculated cross sections along the diagonal \( \theta_A = \theta_B \) are shown by the lighter curves.

Figure 4 shows the \( E_0 = 250 \) eV, \( E_A = 186.4 \) eV, \( E_B = 50 \) eV, \( \phi_A - \phi_B = \pi \) data compared with different calculations. The experimental data have been reported by us previously (Weigold et al 1977). In the figure the data are normalised to give the same peak height as the DWIA-1 cross section for \( \theta_A = 25^\circ \). All the different theoretical calculations are similarly normalised to this peak height in the \( \theta_A = 25^\circ \) angular correlation. The errors shown in the figure are only the statistical errors and do not include the error in determining the relative cross sections at different \( \theta_A \). The total error will be a combination of the two errors given in table 1.

The two plane-wave approximations are obviously completely inadequate, whereas the calculations using the two distorted-wave models give an excellent description of all the data. The plane-wave cross sections are much too large at small \( \theta_A \) (especially at small \( \theta_B \)) and far too small at large \( \theta_A \). Over the measured range of \( \theta_A \) \( (15^\circ - 35^\circ) \) the

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**Figure 4.** The H(e, 2e)\( H^+ \) differential cross section (in units of \( \frac{2}{3} a_0^2 \text{Ryd}^{-1} \text{sr}^{-2} \)) at \( E_0 = 250 \) eV, \( E_B = 50 \) eV, \( E_A = 186.4 \) eV, \( \phi_A - \phi_B = \pi \), plotted as a function of \( \theta_A \) and \( \theta_B \). The calculated cross sections are: ---, DWIA-1; --, DWIA-4 \( \times 1.38 \); ---, PWIA \( \times 0.54 \); ---, PWBE \( \times 0.25 \). The data and calculations are normalised to the peak height of the \( \theta_A = 25^\circ \) DWIA-1 differential cross section. The experimental data are from Weigold et al (1977).
momentum transfer $K_{0A}$ ranges from $1.2a_0^{-1}$ to $2.5a_0^{-1}$ (see table 2). The PWBE cross sections are again approximately a factor of 2 greater than the PWIA cross sections at all angles.

Table 2. Summary of the momentum transfer $K_{0A} = |k_0 - k_A|$ and the angle of momentum transfer $\theta_{0A}$. $\theta_{B,\text{max}}$ indicates the angle $\theta_B$ at which the measured cross section peaks.

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<th>$E_B$(eV)</th>
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<th>$\theta_{B,\text{max}}$(deg)</th>
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Using an effective charge of $-1$ for both $Z_A$ and $Z_B$ (DWIA-1) gives an excellent description of all of the data. Nearly as good is the DWIA-4 model. This is the model in which both the ingoing and fast outgoing electron waves are distorted by the optical potential (equation (10)), the slow outgoing electron wave being a Coulomb wave ($Z_B = -1$). Since this model treats the fast outgoing electron roughly on an equivalent footing to the incident electron, it can only be justified for kinematical conditions such as in this case for which $E_0 \approx E_A \gg E_B$.

Although the optical model is energy dependent, it assumes that the hydrogen atom is in the ground state in the incident and exit channels, instead of being in an excited (continuum) state in the exit channel. It therefore is not consistent with time-reversal invariance. The effect of absorption in the exit channel can be seen in figure 4, the DWIA-4 cross sections being significantly smaller than the DWIA-1 cross sections, the normalisation factor being 1.34.

The data at 113.6 eV are compared with the DWIA-1, PWIA, and PWBE cross sections in figure 5. The errors shown in the figure again do not include the error in determining the differential cross sections at $\theta_A = 35^\circ$ relative to the differential cross section at $\theta_A = 45^\circ$ ($\sigma_N$ in table 1). The experimental data and theoretical cross sections have all been normalised to give the same peak height as the DWIA-1 cross section for $\theta_A = 35^\circ$. The PWBE peak cross sections are more than six and four times the peak magnitudes of the DWIA-1 and PWIA cross sections respectively. Although the DWIA-1 calculations give the best description of the data, it nevertheless does not give an adequate description at large $\theta_{AB}$, i.e. large $K_{0A}$ (or $K_{0B}$ since electrons A and B are completely equivalent in this case).
Figure 5. The \(H(e, 2e)H^+\) differential cross section (in units of \(\frac{1}{2}\alpha_0^2 \text{Ryd}^{-1} \text{sr}^{-2}\)) at \(E_0 = 113.6\text{ eV}, E_A = E_B = 50\text{ eV}, \phi_A - \phi_B = \pi\) plotted as a function of \(\theta_A\) and \(\theta_B\). The calculated cross sections are: \(--\), DWIA-1; \(-\--\), PWIA (\(\times 0.6\)); \(\cdot\cdot\cdot\cdot\), PWBE (\(\times 0.15\)). The data and calculations are normalised to the peak height of the \(\theta_A = 45^\circ\) DWIA-1 differential cross section.

Figure 6 shows the \(E_0 = 100\text{ eV}, E_A = 50\text{ eV}, E_B = 36.4\text{ eV}\) data at \(\theta_A = 20^\circ, 30^\circ\) and \(40^\circ\) compared with the DWIA-1, PWIA and PWBE cross sections. At each \(\theta_A\) the data and two plane-wave theories have all been normalised to the peak height of the DWIA-1 cross section, and therefore only shape comparisons are relevant. The plane-wave theories give cross section shapes in marked disagreement with the measured cross sections, especially at \(\theta_A = 20^\circ\) and \(30^\circ\). The plane-wave theories predict maxima at angles \(\theta_B\) much smaller than the observed \(\theta_{B,\text{max}}\) (table 2). The DWIA-1 approximation on the other hand gives cross section shapes in excellent agreement with the data, although at \(\theta_A = 40^\circ\) it moves the maximum in the cross section to an angle \(\theta_B\) somewhat larger than the observed \(\theta_{B,\text{max}}\). Once again the introduction of distorted waves in the incident channel and Coulomb waves in the exit channel reduces the calculated cross sections considerably. It should also be noted that the plane-wave Born cross sections are more than four times those of the PWIA under these kinematical conditions, and a relatively crude absolute measurement could distinguish between the PWBE, PWIA and DWIA models.

The data at \(E_0 = 100\text{ eV}, E_A = 61.4\text{ eV}, E_B = 25\text{ eV}\) and \(\theta_A = 20^\circ\) and \(30^\circ\) are shown in figures 7 and 8 respectively. Also shown in the figures are four different DWIA calculations as well as the PWIA and PWBE calculations. The data and the cross sections given by the different approximations have all been normalised to give the same peak
heights as the DWIA-1 cross sections. The different multiplication factors are again indicated in the figures.

The two plane-wave theories are again totally inadequate, although the impulse approximation does considerably better than the PWBE model. The cross section maxima given by the PWBE are at angles much smaller than the measured maxima, whereas the PWIA maxima are in much better agreement with the data. The PWBE cross sections are again approximately four times the PWIA cross sections, and at OA = 20° (figure 7) they are more than an order of magnitude greater than the DWIA-1 cross sections.

The DWIA-1 approximation, with ZA = ZB = -1 shifts the cross section maximum too large an angle at OA = 20° (figure 7), although it provides an adequate description of the data at OA = 30°.

The DWIA-2 model has the effective charges ZA and ZB determined by equation (17). These effective charges, which are consistent with the asymptotic condition of equation (13), depend on the angles OA and OB. At OA = 20° they range from ZA = +0.31, and ZB = -1.0 at OB = 30° to ZA = -0.31, ZB = -0.85 at OB = 60° (close to the maximum in the observed cross section), and at OB = 90° they are ZA = -0.51 and ZB = -0.84. At OA = 30° the values are ZA = 0, ZB = -0.92 at OB = 30°; ZA = -0.31,
Figure 7. The H(e, 2e)H⁺ differential cross section (in units of \( \frac{1}{2}a_0^2 \text{ Ryd}^{-1} \text{ sr}^{-2} \)) at \( E_o = 100 \text{ eV}, E_A = 61.4 \text{ eV}, E_B = 25 \text{ eV}, \theta_A = 20° \) plotted as a function of \( \theta_B \). The data at \( \phi_A - \phi_B = \pi \) and 0 are indicated by \(^{\circ}\) and \(^{\circ}\) respectively. The calculated cross sections are: 

- DWIA-1; 
- DWIA-2 (\( \times 0.46 \)); 
- DWIA-3 (\( \times 0.46 \)); 
- PWIA (\( \times 1.34 \)); 
- PWBE (\( \times 0.04 \)).

The data and calculations have been normalised to the DWIA-1 peak height. At angles \( \theta_B > 50° \) the DWIA-2 and DWIA-3 models are nearly indistinguishable and only the DWIA-2 curve is shown.

\( Z_B = -0.85 \) at \( \theta_B = 50° \) (near the cross section maximum); and at \( \theta_B = 90° \), \( Z_A = -0.55 \), \( Z_B = -0.84 \).

Thus in DWIA-2 the effective charge of the ‘slow’ electron is always close to \(-1\), while the effective charge on the ‘fast’ electron varies much more and is even positive for small angles \( \theta_B \). At one angle (\( \theta_{AB} \approx 60° \)) \( Z_A \) is actually zero, and the electron wave \( \chi_A^{(s)} \) is simply a plane wave. These effective charges can be easily understood in the spirit of the asymptotic arguments. The fast electron A soon leaves the interaction region far behind, the slow electron B being always much closer to the proton than to the fast electron. Thus at large distances the fast electron ‘sees’ a neutral system of electron B plus the proton and hence has a small effective charge, while the slow electron will to a large extent only see the close-by proton, and hence will have an effective charge of approximately \(-1\). The effective charge \( Z_A \) of the fast electron also depends sensitively on the relative angle of emission \( \theta_{AB} \), i.e. on whether electron B or the proton is the nearer particle. Of course these asymptotic arguments may not lead to the correct description in the region where the electrons and proton are all in close proximity. This is best illustrated by noting that equation (17) leads to a value of \( Z_A = 0 \), \( Z_B \approx -1 \), at certain angles, that is the faster outgoing wave can be a plane wave even though its energy (61.4 eV) is well below that of the incident electron, whose wavefunction is fully distorted by the optical potential.
Figure 8. As for figure 7 except $\theta_A = 30^\circ$ and $\phi_A - \phi_B = \pi$ for all the data. The calculated cross sections are: ——, DWIA-1; . . . , DWIA-2 ($\times 0.67$); · · · , DWIA-3 ($\times 0.67$); — —, DWIA-4 ($\times 1.14$); — — —, PWIA ($\times 0.46$); — — , PWBE ($\times 0.13$).

The DWIA-2 approximation gives cross sections which are intermediate in magnitude between those of the DWIA-1 and PWIA models. This could be expected on the basis that the effective charges are intermediate between the respective extremes of $-1$ and $0$. The cross section shape is however very much closer to that of the PWIA, being almost indistinguishable at $\theta_A = 30^\circ$ (figure 8). At both $\theta_A = 20^\circ$ and $30^\circ$ (figures 7 and 8) the DWIA-2 model considerably enhances the small angle ($\theta_B$) cross section, even over that given by the PWIA model.

The effect of fixing the effective charges at some average value is investigated in the DWIA-3 calculations. The effective charges given by equation (17) at approximately the maxima in the cross sections are used at all angles. They are $Z_A = -0.31$ and $Z_B = -0.85$ at both $\theta_A$ values. Figures 7 and 8 show that the effect of fixing the effective charges considerably reduces the cross sections at small values of $\theta_B$ in agreement with experiment, while leaving the cross section at the larger angles relatively unchanged. Where the two cross sections are not significantly different, only one (DWIA-2) is shown on figures 7 and 8. From a comparison of the DWIA-1, 2 and 3 cross sections it is apparent that at small $\theta_B$, lowering the magnitude of the effective charges leads to a marked increase in the relative cross section, while at large $\theta_B$ it leads to a reduction in the cross section. As in figure 4, the experiments indicate that the effective charges should decrease with angle, rather than increase as given by equation (17).

The DWIA-4 cross sections are also shown in figures 7 and 8. This approximation should also be applicable in this case since $E_A$ is considerably greater than $E_B$. $Z_A = 0$
and $Z_B = -1$ in this approximation but $\chi_A^{(-1)}$ is fully distorted. It gives an excellent description of the small angle cross section, but at $\theta_A = 30^\circ$ it considerably underestimates the cross section at angles $\theta_B > 60^\circ$. At $\theta_A = 20^\circ$ it gives an adequate description of all the data except at $\theta_B > 100^\circ$, where it predicts a rise in the cross section which is not observed. None of the DWIA models adequately describes all of the data at $\theta_A = 20^\circ$ and $30^\circ$.

5. Summary and conclusions

We have shown that the measurement of $H(e, 2e)H^+$ cross sections in the intermediate energy region provides a very sensitive test of ionisation theories, being particularly sensitive to correlation effects in the final state. The experiments are compared with various factorised distorted-wave half-off-shell impulse approximations, the PWIA and PWBE approximation. The different distorted-wave approximations differ only in their treatment of the two outgoing electron waves. In DWIA-1 the emitted electron waves are Coulomb waves of full effective charge ($-1$), in DWIA-2 the effective charges depend on the angles of emission and are determined by asymptotic constraints (equations (19, (17)), DWIA-3 uses a constant average effective charge for each electron, and finally in DWIA-4 the slow emitted electron has an effective charge of $-1$ and the fast electron is a distorted wave, the distorting potential being the energy-dependent ground-state optical potential.

The two plane-wave approximations are completely inadequate at all energies ($E_0 = 100-413.6$ eV). The PWIA gives a somewhat better description of the data. The distorted-wave approximations, even though they involve the additional factorisation approximation (equation (5)), give much improved fits to the data.

The approximation with effective charges $Z_A = Z_B = -1$ is obviously better than that with effective charges consistent with the asymptotic constraint. This is particularly so at low $K_{OA}$ ($\leq 2a_0^{-1}$). At higher $K_{OA}$ ($\geq 3a_0^{-1}$), i.e. at larger angles $\theta_A$ (and $\theta_B$), effective charges somewhat smaller in magnitude than unity give a better description of the data. This angular dependence of the effective charges is just the opposite to that predicted by the asymptotic conditions (equations (15) and (17)), which require the magnitudes of the effective charges to decrease as the angle $\theta_{AB}$ decreases. This is due to the screening of the proton charge at small angles. At large angles of emission the proton charge is not effectively screened by the other electron and $Z_A \approx Z_B \approx -1$.

When the two electrons and proton are in close proximity and interacting strongly, the use of asymptotic arguments to determine the electron wavefunctions is likely to be inappropriate. This can be seen from a semiclassical argument. Large momentum transfer signifies close electron–electron collisions, i.e. small impact parameters $\tilde{r}_{OA}$. For $K_{OA} \sim 4a_0^{-1}$, $\tilde{r}_{OA} \sim a_0/4$ and the electrons are on average closer to each other than to the proton at their point of strongest interaction. The proton charge is therefore on average shielded to some degree by the other electron, and their effective charges are correspondingly reduced. The asymptotic picture gives the opposite result, i.e. at large $K_{OA}$ the electrons emerge at large angles relative to each other and the proton charge is essentially unshielded. On the other hand for small $K_{OA} (\ll a_0^{-1})$, $\tilde{r}_{OA}$ is large ($\gg a_0$), and the proton is essentially unshielded at the point of 'closest approach' and $Z_A$ and $Z_B$ should be large in magnitude ($\approx -1$). Asymptotically, as the electrons move to large distances from the proton, a small angle of emission $\theta_{AB}$ implies of course that the magnitude of the effective charges should be correspondingly reduced. The data are
essentially in agreement with this crude semiclassical argument and show that asymptotic constraints give the wrong effective charges in the model using Coulomb waves for the two final-state electrons.

When \( E_0 = E_A \gg E_B \) it may be appropriate to ignore the escape velocity of the slow emitted electron and treat the outgoing wave as a distorted wave in an analogous way to the incident electron. The wavefunction of the slow electron is then obviously a Coulomb wave with effective charge \( Z_B = -1 \). The distorted waves \( \chi_{\omega\lambda}^j \) are calculated using the appropriate energy-dependent optical-model potential for scattering by ground-state hydrogen. Besides containing static, exchange and polarisation terms, the imaginary part gives rise to absorption. This model, since it contains absorption in both incident and exit channels, gives the smallest (e, 2e) cross sections. In the two cases most appropriate to this model \( (E_0 = 250 \text{ eV}, \ E_B = 50 \text{ eV} \) and \( E_0 = 100 \text{ eV}, \ E_B = 25 \text{ eV} \) it gives a very good description of the data.

Although the factorised distorted-wave models all give a very much improved description of the data compared to the plane-wave theories, none of them give a completely adequate description of the data at all energies and angles. The calculated cross sections are extremely sensitive to the choice of the wavefunctions of the emitted electrons. The overall agreement between the data and the DWIA calculations argues that the factorisation approximation is adequate. It would nevertheless be interesting to compare the measured differential cross sections with distorted-wave Born-approximation calculations using realistic distorted waves, since in the DWBA model the factorisation approximation need not be made. In the light of the large differences in magnitude between the PWIA and PWBE cross sections, and between the DWIA and DWBA (C J Noble and J Smith 1978, private communication), reasonably accurate absolute measurements should be able to discriminate between the half-off-shell impulse and Born approximations.

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**References**