

## Electron scattering by atomic hydrogen: the distorted-wave second Born approximation

A E Kingston and H R J Walters

Department of Applied Mathematics and Theoretical Physics, The Queen's University of Belfast, Belfast, BT7 1NN, Northern Ireland

Received 2 June 1980, in final form 25 July 1980

**Abstract.** The distorted-wave second Born approximation (DWSBA) has been applied to the elastic scattering of electrons by ground-state atomic hydrogen and to the electron impact excitation of the  $1s \rightarrow 2s$  and  $1s \rightarrow 2p$  transitions in the energy range 30 to 680 eV. Differential and total cross sections are given as well as the polarisation fraction of the Lyman  $\alpha$  radiation resulting from the radiative transition  $2p \rightarrow 1s$ . A new method of choosing the average energy in the closure approximation to the second Born amplitude is introduced for elastic scattering. The approximate methods of Dewangan and Walters and Winters for including distortion effects in the second Born term are investigated. It is found that both approximations are viable for elastic scattering at high enough energies but unreliable for inelastic scattering. Since the Winters approximation is based upon a local second-order potential this result spells out a warning to all those working with such potentials. The DWSBA differential cross sections for elastic scattering are in fairly good agreement with the experimental data of Williams. This agreement is consistent with previous work on He and Ne. However, the DWSBA is found to be in poor accord with the  $n = 2$  excitation cross sections of Williams and Willis. It is suggested that new independent measurements of these cross sections might be in order.

### 1. Introduction

If perturbation theory is to be applied to a problem it must be applied sensibly. At the outset it must be decided which aspects of the problem, if any, can be treated perturbatively and which cannot. This division of the problem into perturbative and non-perturbative components leads, in the case of scattering theory, to the division of the interaction potential  $V$  into two parts:  $V_2$  which is amenable to perturbation theory and  $V_1$  which must be handled more carefully. Having made such a separation of the interaction the ploy is now to obtain a perturbation expansion of the scattering amplitude in powers of  $V_2$  but such that  $V_1$  is always treated exactly. This idea leads to the so-called distorted-wave Born series.

The above philosophy has been applied with some success to the elastic scattering of electrons by He and Ne at intermediate and high energies (Dewangan and Walters 1977). Here it seems adequate, at least for the direct scattering amplitude, to work only to second order in  $V_2$  (the distorted-wave second Born approximation (DWSBA)), indeed the lowness of the order in  $V_2$  required is a measure of the effectiveness of the separation of  $V$  into perturbative and non-perturbative parts. Only one application of the DWSBA to electron impact excitation is known to us, this is the work of Winters

(1978) on the  $1s \rightarrow 2s$  excitation of atomic hydrogen. However, this work was more qualitative than quantitative, a rather crude closure approximation having been used in the second Born term. In this paper we make a careful study of the DWSBA to the elastic scattering of electrons by atomic hydrogen and also to the electron impact excitation of the  $2s$  and  $2p$  states.

In the application of the DWSBA to electron-atom scattering two major technical problems arise. The first is how to evaluate the sum over all target states in the second Born term and the second is how to employ distorted waves in this same term.

The first of these problems has a long history. The normal solution to it, today, is to employ the simplified second Born approximation of Holt and Moiseiwitsch (1968). In this approximation the contributions of a number of 'important' states are calculated exactly, the remaining states are then included by assigning to them an average energy  $\bar{\epsilon}$ . This last trick enables the completeness property of the target states to be exploited to reduce the second Born term to a reasonably tractable form. Clearly there are two fundamental questions we must ask about this approximation: (i) is it quantitatively viable? (ii) if so, what is a good choice for  $\bar{\epsilon}$ ? From the evidence we have, which includes an exact calculation of the (plane-wave) second Born amplitude for elastic electron-hydrogen scattering at 30 eV (Ermolaev and Walters 1979), the answer to this first question seems to be in the affirmative, at least for elastic scattering at intermediate to high energies. The second question is one of the main concerns of the present paper. In particular, for elastic scattering we introduce a brand new approach to the determination of  $\bar{\epsilon}$  whose usefulness has been confirmed by the exact results of Ermolaev and Walters<sup>†</sup>.

The technical difficulties associated with using distorted waves in the second Born term have led to the use of approximations. At first it was thought, hopefully, that plane waves might be good enough for the second-order term (Buckley and Walters 1974, 1975). However Dewangan and Walters (1977) showed that distorted waves really had to be used in order to realise the full potential of the DWSBA. They suggested an 'on-energy-shell' approximation for including distortion in the second Born term. While the excellent agreement they obtained with experiment at the higher energies seems to justify their approximation it is still important that it be rigorously checked, if only to remove any slight doubt that the agreement obtained may have been fortuitous. In his work on the  $1s \rightarrow 2s$  transition in hydrogen Winters (1978) used a local potential approximation to include distortion effects; this potential was generated by Fourier transforming the plane-wave second Born amplitude (again, essentially, an 'on-energy-shell' approximation), Bransden *et al* (1978) claim to have verified Winters approximation for elastic  $e^-$ -He scattering within their second-order potential method, but no test has been made for inelastic scattering.

In this paper we evaluate the effects of distortion in the second Born term exactly. This enables us to test the Dewangan-Walters approximation and the Winters local potential method rigorously, both for elastic scattering and for the  $1s \rightarrow 2s$  and  $1s \rightarrow 2p$  excitations. We find that both approximations are justified, Winters' the more so, for elastic scattering, but both fail for inelastic scattering. In view of the interest in local second-order potentials (see, for example, Furness and McCarthy 1973, Vanderpoorten 1975, Byron and Joachain 1977b, McDowell 1980) the failure of the Winters' method for inelastic scattering is an important result.

<sup>†</sup> The present paper is that referenced by Ermolaev and Walters as 'Kingston and Walters (1979) to be published'.

Our DWSBA results for elastic electron-hydrogen scattering are in fairly good agreement with experiment. When placed together with the previous work on He and Ne (Dewangan and Walters 1977) definite common patterns can be discerned; for example, the breakdown mode of the DWSBA at low energies. Such pattern recognition over a range of atoms enables us to make very definite statements about disagreement between theory and experiment in particular cases. Thus, for example, we are able to say with some confidence that the experimental data of Williams (1975) at 100 eV are in error.

The DWSBA results for the excitation reactions  $1s \rightarrow 2s$  and  $1s \rightarrow 2p$  are in disappointing agreement with the measurements of Williams and Willis (1975). It is not clear to us which of the two is in error. Further independent measurements of the  $n = 2$  excitation cross section would be very useful; so also would further experience with the DWSBA on other atomic systems to see if a pattern of agreement (or disagreement) between theory and experiment can be established.

Throughout this paper we use atomic units in which  $\hbar = m_e = e = 1$ . The symbol  $a_0$  denotes the Bohr radius.

## 2. The distorted-wave second Born approximation—theory and practice

We consider the scattering of an electron with wave vector  $\mathbf{k}_0$  incident upon a hydrogen atom in the state  $\psi_0$ . If the electron emerges with wave vector  $\mathbf{k}_f$  and the atom is left in the state  $\psi_f$ , then, ignoring electron exchange effects, the direct scattering amplitude for this process is

$$f_{0f}(\mathbf{k}_f, \mathbf{k}_0) = -\frac{1}{2\pi} \langle \mathbf{k}_f, \psi_f | V | \Psi^+ \rangle \quad (1)$$

where

$$V = \frac{1}{|\mathbf{r}_1 - \mathbf{r}_0|} - \frac{1}{r_0} \quad (2)$$

$$\langle \mathbf{k}_f, \psi_f | V | \Psi^+ \rangle \equiv \int \exp(-i\mathbf{k}_f \cdot \mathbf{r}_0) \psi_f^*(\mathbf{r}_1) V \Psi^+(\mathbf{r}_0, \mathbf{r}_1) d\mathbf{r}_0 d\mathbf{r}_1. \quad (3)$$

Here  $\mathbf{r}_0$  and  $\mathbf{r}_1$  are the coordinates of the incident and atomic electrons respectively, \* denotes complex conjugation, and  $\Psi^+$  is the complete scattering wavefunction for the system.

Splitting  $V$  into two parts

$$V = V_1 + V_2 \quad (4)$$

the amplitude (1) may be expanded in a power series in  $V_2$ , the distorted-wave Born series (see Dewangan and Walters 1977)

$$\begin{aligned} f_{0f}(\mathbf{k}_f, \mathbf{k}_0) = & -\frac{1}{2\pi} \langle \mathbf{k}_f, \psi_f | V_1 | \Phi_0^+(\mathbf{k}_0) \rangle \\ & - \frac{1}{2\pi} \langle \Phi_f^-(\mathbf{k}_f) | (V_2 + V_2 G_1^+ V_2 + V_2 G_1^+ V_2 G_1^+ V_2 + \dots) | \Phi_0^+(\mathbf{k}_0) \rangle \end{aligned} \quad (5)$$

where

$$\Phi_t^\pm(\mathbf{k}) = \exp(i\mathbf{k} \cdot \mathbf{r}_0)\psi_t + G_0^\pm V_1 \Phi_t^\pm(\mathbf{k}) \quad (t = 0 \text{ or } f) \quad (6)$$

$$G_0^\pm = \lim_{\eta \rightarrow 0+} (E - H_0 \pm i\eta)^{-1} \quad (7)$$

$$G_1^\pm = \lim_{\eta \rightarrow 0+} (E - H_0 - V_1 \pm i\eta)^{-1} \quad (8)$$

$E$  is the total energy and  $H_0$  is the sum of the kinetic energy operator for the incident electron and the atomic Hamiltonian.

Even though the whole interaction  $V$  may not be suitable for perturbative treatment it may be that an important part of it is. In our notation this part is represented by  $V_2$ , while  $V_1$  contains those properties which render  $V$  unsatisfactory for a perturbative calculation. To exploit this division of  $V$  we require a power series expansion of the scattering amplitude in terms of  $V_2$ , an expansion in which  $V_1$  is treated non-perturbatively, i.e. exactly. This is provided by the distorted-wave Born series (5).

The situation envisaged in the previous paragraph is believed to exist in electron-atom scattering (Buckley and Walters 1974, 1975, Walters 1976a, Dewangan and Walters 1977). The principal property of the potential (2) which makes it unsuitable for perturbation treatment is the singular electron-nucleus interaction  $-r_0^{-1}$  (Dewangan and Walters 1977). The primary aim in dividing  $V$  must therefore be to place this electron-nucleus term in  $V_1$ . In practice only part of the electron-nucleus interaction is normally included in  $V_1$ —the most important part, we think.

Following precedent (Buckley and Walters 1974, Walters 1976a, Dewangan and Walters 1977) we take

$$V_1 = PVP \quad (9)$$

where the operator  $P$  projects onto a finite subspace of bound atomic states  $\psi_n$  (of unit norm) which includes both  $\psi_0$  and  $\psi_f$ , i.e.

$$P = \sum_{n=0}^N |\psi_n(\mathbf{r}_1)\rangle \langle \psi_n(\mathbf{r}_1)|. \quad (10)$$

Scattering by  $V_1$  can then be obtained exactly by solving a system of  $(N+1)$  close-coupled equations. The choice (9) and (10) does not totally eliminate the electron-nucleus term from  $V_2$ . It does, however, allow exactly for scattering of the electron by the static potentials,  $\langle \psi_0(\mathbf{r}_1) | V | \psi_0(\mathbf{r}_1) \rangle$  and  $\langle \psi_f(\mathbf{r}_1) | V | \psi_f(\mathbf{r}_1) \rangle$ , of the initial and final states of the target atom; it is in this scattering that the electron-nucleus interaction makes itself most strongly felt.

Choosing  $V_1$  according to (9) and (10), and keeping only terms up to second order in  $V_2$ , we obtain the following distorted-wave second Born approximation to (5)

$$f_{0f}(\mathbf{k}_f, \mathbf{k}_0) = f_{0f}^{\text{cc}}(\mathbf{k}_f, \mathbf{k}_0) - \frac{1}{2\pi} \langle \Phi_f^-(\mathbf{k}_f) | V_2 G_0^+ V_2 | \Phi_0^+(\mathbf{k}_0) \rangle \quad (11)$$

where  $f_{0f}^{\text{cc}}$  is the scattering amplitude calculated in the (non-exchange)  $(N+1)$  state  $(\psi_0, \psi_1, \dots, \psi_N)$  close-coupling approximation. The approximation (11) forms the basis of the present work.

Expanding the wavefunctions  $\Phi_0^+$  and  $\Phi_f^-$  in the (complete) basis  $\psi_0, \psi_1, \dots, \psi_N$  i.e.

$$\Phi_t^\pm = \sum_{n=0}^N F_{tn}^\pm(\mathbf{r}_0)\psi_n(\mathbf{r}_1) \quad (t = 0 \text{ or } f) \quad (12)$$

the second-order term in (11) may be written

$$\langle \Phi_f^-(\mathbf{k}_f) | V_2 G_0^+ V_2 | \Phi_0^+(\mathbf{k}_0) \rangle = \sum_{p,q=0}^N \langle F_{fp}^-, \psi_p | V_2 G_0^+ V_2 | F_{0q}^+, \psi_q \rangle. \quad (13)$$

For our 1s → 1s elastic scattering calculations we have taken  $P$  (see (10)) to be simply

$$|\psi_{1s}(\mathbf{r}_1)\rangle\langle\psi_{1s}(\mathbf{r}_1)|. \quad (14)$$

In this case, using (13), the expression (11) becomes

$$f_{1s,1s}(\mathbf{k}_f, \mathbf{k}_0) = f_{1s,1s}^{\text{cc}}(\mathbf{k}_f, \mathbf{k}_0; 1s) - \frac{1}{2}\pi^{-1} \langle F_{1s,1s}^-, \psi_{1s} | V_2 G_0^+ V_2 | F_{1s,1s}^+, \psi_{1s} \rangle \quad (15)$$

where  $f_{1s,1s}^{\text{cc}}(\mathbf{k}_f, \mathbf{k}_0; 1s)$  is the scattering amplitude in the static field (i.e. one-state non-exchange close-coupling) approximation.

For the 1s → 2s excitation we have chosen  $P$  to be

$$|\psi_{1s}(\mathbf{r}_1)\rangle\langle\psi_{1s}(\mathbf{r}_1)| + |\psi_{2s}(\mathbf{r}_1)\rangle\langle\psi_{2s}(\mathbf{r}_1)|. \quad (16)$$

Again using (13) we obtain for (11)

$$\begin{aligned} f_{1s,2s}(\mathbf{k}_f, \mathbf{k}_0) = & f_{1s,2s}^{\text{cc}}(\mathbf{k}_f, \mathbf{k}_0; 1s+2s) - \frac{1}{2}\pi^{-1} \langle F_{2s,1s}^-, \psi_{1s} | V_2 G_0^+ V_2 | F_{1s,1s}^+, \psi_{1s} \rangle \\ & + \langle F_{2s,2s}^-, \psi_{2s} | V_2 G_0^+ V_2 | F_{1s,1s}^+, \psi_{1s} \rangle + \langle F_{2s,1s}^-, \psi_{1s} | V_2 G_0^+ V_2 | F_{1s,2s}^+, \psi_{2s} \rangle \\ & + \langle F_{2s,2s}^-, \psi_{2s} | V_2 G_0^+ V_2 | F_{1s,2s}^+, \psi_{2s} \rangle \end{aligned} \quad (17)$$

where  $f_{1s,2s}^{\text{cc}}(\mathbf{k}_f, \mathbf{k}_0; 1s+2s)$  is the scattering amplitude in the non-exchange two-state 1s–2s close-coupling approximation. Consideration of the second-order amplitudes in (17) leads us to believe that the second term in the bracket of (17) will be more important than the other three; for example, this would be the only non-zero term if the unperturbed functions  $\exp(i\mathbf{k} \cdot \mathbf{r}_0)\psi_i$  were used for  $\Phi_i^\pm(k)$  (see (6)). We have therefore introduced a further approximation, the neglect of the remaining three amplitudes. Formula (17) then reduces to

$$f_{1s,2s}(\mathbf{k}_f, \mathbf{k}_0) = f_{1s,2s}^{\text{cc}}(\mathbf{k}_f, \mathbf{k}_0; 1s+2s) - \frac{1}{2}\pi^{-1} \langle F_{2s,2s}^-, \psi_{2s} | V_2 G_0^+ V_2 | F_{1s,1s}^+, \psi_{1s} \rangle. \quad (18)$$

First-order distorted-wave theories of excitation which employ distorted waves calculated using second-order elastic scattering optical potentials in the initial and final channels (Joachain and Vanderpoorten 1973, Madison 1980) take into account a substantial part of the first and fourth terms in the bracket of (17)<sup>†</sup>. The results of such calculations (Joachain and Vanderpoorten 1973) suggest, although not without ambiguity, that the first and fourth terms (and perhaps their higher order iterations) may not be totally unimportant at lower energies. While a careful examination of these terms would be of interest it is important first to make a rigorous study of the more dominant second-order amplitude retained in (18); this we do in the present work.

The choice of  $P$  for the 1s → 2p excitation was

$$|\psi_{1s}(\mathbf{r}_1)\rangle\langle\psi_{1s}(\mathbf{r}_1)| + \sum_{m=-1,0,+1} |\psi_{2p_m}(\mathbf{r}_1)\rangle\langle\psi_{2p_m}(\mathbf{r}_1)|. \quad (19)$$

Using this in (11), and making a further approximation analogous to that in the 1s → 2s

<sup>†</sup> The reader will recognise  $\langle \psi_{1s} | V_2 G_0^+ V_2 | \psi_{1s} \rangle$  as being an elastic scattering second-order optical potential in the 1s channel; similarly  $\langle \psi_{2s} | V_2 G_0^+ V_2 | \psi_{2s} \rangle$ .

case, i.e. the neglect of all terms in (13) except  $q = 1s$  and  $p = 2p_{-1}, 2p_0, 2p_{+1}$ , we obtain†

$$f_{1s,2p_m}(k_f, k_0) = f_{1s,2p_m}^{cc}(k_f, k_0; 1s + 2p) - \frac{1}{2\pi} \sum_{\mu=-1,0,+1} \langle F_{2p_m,2p_\mu}^- | \psi_{2p_\mu} | V_2 G_0^+ V_2 | F_{1s,1s}^+ | \psi_{1s} \rangle \quad (20)$$

where  $f_{1s,2p_m}^{cc}(k_f, k_0; 1s + 2p)$  is the scattering amplitude in the non-exchange 1s–2p close-coupling approximation.

To take account of electron exchange effects, which we have so far ignored, we replace the non-exchange close-coupling amplitudes in (15), (18) and (20) by amplitudes calculated in the corresponding close-coupling approximations *with exchange*. Analogous to (12) the associated spatial wavefunctions may be expanded as

$$\Phi_i^{\pm(1)} = \sum_{n=0}^N (F_{in}^{\pm(1)}(r_0)\psi_n(r_1) + F_{in}^{\pm(1)}(r_1)\psi_n(r_0)) \quad (21a)$$

$$\Phi_i^{\pm(3)} = \sum_{n=0}^N (F_{in}^{\pm(3)}(r_0)\psi_n(r_1) - F_{in}^{\pm(3)}(r_1)\psi_n(r_0)) \quad (21b)$$

where 1 labels the singlet wavefunction and 3 the triplet.

It would also be desirable, we feel, to replace the non-exchange distorted waves  $F_{in}^{\pm}$  in the second-order terms of (15), (18) and (20) by their with-exchange counterparts  $F_{in}^{\pm(1),(3)}$ . However, a disadvantage in making this substitution is that the second-order amplitudes in (15), (18) and (20) would have to be calculated twice, once for singlet scattering and again for triplet scattering. We have therefore employed the (easily implemented) prescription of Dewangan and Walters for including distortion‡ (see § 4) to investigate how much change would, in fact, be produced by such a replacement. Our results indicated that the change would be very small for the excitation reactions  $1s \rightarrow 2s$  and  $1s \rightarrow 2p$  in the energy range of interest to us (54.4 eV upwards). The  $1s \rightarrow 1s$  elastic scattering process was a bit more sensitive: at the two lowest energies we consider, i.e. 30 and 50 eV, there was a noticeable change. However, beyond 100 eV the elastic scattering results were also insensitive to the replacement. In treating the  $1s \rightarrow 2s$  and  $1s \rightarrow 2p$  excitations we have therefore used only the non-exchange distorted waves  $F_{in}^{\pm}$  in the second-order amplitudes of (18) and (20)§. For elastic scattering, on the other hand, we have made the substitution  $F_{1s1s}^{\pm} \rightarrow F_{1s,1s}^{\pm(1),(3)}$  in (15)¶.

In the present paper we shall attach the name distorted-wave second Born approximation (DWSBA) to results calculated from the amplitudes (15), (18) and (20), modified for electron exchange as described above.

† Note that this time we do keep some second-order amplitudes, i.e.

$$\langle F_{2p_m,2p_\mu}^- | \psi_{2p_\mu} | V_2 G_0^+ V_2 | F_{1s,1s}^+ | \psi_{1s} \rangle$$

( $\mu \neq m$ ), which would be zero when unperturbed functions are used for the  $\Phi_i^{\pm}$ . It is here computationally convenient to do so.

‡ Although this is not, in general, a perfectly accurate approximation, it should, nevertheless, accurately reflect the magnitude of the change we are examining here.

§ We emphasise that the close-coupling amplitudes,  $f^{cc}$ , are still calculated with full allowance for exchange.

¶ A minor dilemma arises in connection with the triplet distorted waves  $F_{in}^{\pm(3)}$ . From (21b) it is clear that the  $F_{in}^{\pm(3)}$  are not unique, since  $\Phi_i^{\pm(3)}$  is unchanged when any  $F_{in}^{\pm(3)}$  is replaced by  $F_{in}^{\pm(3)} + \alpha\psi_n$  ( $\alpha$  any constant). In our calculations we have fixed the  $F_{1s,1s}^{\pm(3)}$  by demanding that they be orthogonal to  $\psi_{1s}$ . This is an arbitrary choice, but a reasonable one; the need to make it reflects an inconsistency in our treatment of exchange.

In this work we shall also have cause to refer to the exchange corrected simplified second Born approximation (ECSSBA) of Buckley and Walters (1975). We note here that this approximation differs from our DWSBA only in the replacement of the distorted waves in the second-order amplitudes of (15), (18) and (20) by plane waves. The ECSSBA is easier to calculate than the DWSBA.

Finally, the quantities we calculate, mainly cross sections, are those appropriate to a (spin) unpolarised electron beam incident upon an unpolarised target atom. For example, our differential cross sections are calculated according to

$$\frac{d\sigma}{d\Omega} = \frac{1}{4} \frac{k_f}{k_0} (|f^{(1)}|^2 + 3|f^{(3)}|^2) \quad (22)$$

where  $f$  is the scattering amplitude.

### 3. The simplified second Born approximation

The principal burden of the calculation is the evaluation of second-order terms of the form, see (13),

$$\langle F_p, \psi_p | V_2 G_0^+ V_2 | F_q, \psi_q \rangle \quad (23)$$

where, simplifying notation,  $F_p$  and  $F_q$  are distorted waves. Making a spectral resolution of  $G_0^+$ , remembering the choice (9) and (10) of  $V_1$ , and noting that  $\psi_p$  and  $\psi_q$  belong to the set  $\psi_0, \psi_1, \dots, \psi_N$  (see (13)), (23) may be written

$$\frac{1}{4\pi^3} \sum_{n=N+1}^{\infty} \left( \lim_{\eta \rightarrow 0^+} \int \frac{\langle F_p, \psi_p | V | \mathbf{k}, \psi_n \rangle \langle \mathbf{k}, \psi_n | V | F_q, \psi_q \rangle}{k_n^2 - k^2 + i\eta} d\mathbf{k} \right) \quad (24)$$

where

$$k_n^2 = k_0^2 + 2(\epsilon_0 - \epsilon_n) \quad (25)$$

and  $\epsilon_n$  is the energy of the state  $\psi_n$ .

To evaluate (24) we have adopted, as usual, the simplified second Born approximation of Holt and Moiseiwitsch (1968). In this approximation the contributions from  $M$  'important' intermediate states ( $n = N+1$  to  $N+M$ , say) are calculated exactly, while those from the remaining states are treated approximately by use of an average energy  $\bar{\epsilon}$  (i.e.  $\epsilon_n \rightarrow \bar{\epsilon}$  independent of  $n$ , for  $n \geq N+M+1$ ). The completeness, or closure, property of the states  $\psi_n$  may then be used to render (24) into more tractable form. In the calculations reported here the contributions of 2s and 2p intermediate states, whenever they occur, are always evaluated exactly; all other states are assigned an average energy<sup>†</sup>. The next problem is what to take for  $\bar{\epsilon}$ .

A very important physical effect in electron-atom elastic scattering is target polarisation. It can be shown (Moiseiwitsch 1963) that this is taken into account exactly, and in a dynamic rather than an adiabatic way (Walters 1976b), in the second-order amplitude of (15). A sensible choice for  $\bar{\epsilon}$  would therefore be that which correctly reproduced the target dipole polarisability.

<sup>†</sup> Note that the choices (14), (16) and (19) of  $V_1$  preclude 1s from being an intermediate state in a second-order term.

The polarisation potential for a hydrogen atom in the 1s state is

$$V^{\text{pol}}(r_0) = \sum_{n \neq 1s} \frac{\langle \psi_{1s} | V | \psi_n \rangle \langle \psi_n | V | \psi_{1s} \rangle}{\epsilon_{1s} - \epsilon_n}. \quad (26)$$

The dipole polarisability of the state,  $\alpha_{1s,1s}$ , is defined in terms of the asymptotic form of (26) for large  $r_0$ .

$$V^{\text{pol}} \xrightarrow{r_0 \rightarrow \infty} -\frac{\alpha_{1s,1s}}{2r_0^4}. \quad (27)$$

Consider an approximation to (26) in which the contributions from the states  $n = 0$  to  $n = N + M$  are calculated exactly while an average energy  $\bar{\epsilon}$  is used for the remaining states—this is the analogue of the simplified second Born approximation to (24). The energy  $\bar{\epsilon}$  may now be chosen so that the approximate  $V^{\text{pol}}$  has the correct asymptotic form (27). If this same  $\bar{\epsilon}$  is used in the simplified second Born approximation to the second-order amplitude of (15) then the correct dipole polarisability of the 1s state will be incorporated into that amplitude. This procedure has been adopted by various authors (Moiseiwitsch 1963, Bonham 1971a, b, Bransden and Coleman 1972, Dewangan and Walters 1977). When only the 2s† and 2p states are included exactly in the second-order amplitude of (15),  $\bar{\epsilon}$  must have the value‡

$$\bar{\epsilon} = +0.0779 \text{ au.} \quad (28)$$

The above procedure may be generalised to inelastic scattering. We associate with the second-order amplitudes of (18) and (20) the ‘transition polarisation potentials’ (see, for example, Bransden and Dewangan 1979)

$$V_{2s,1s}^{\text{pol}}(r_0) \equiv \sum_{\substack{\text{all } n \\ \text{except } \epsilon_n = \epsilon}} \frac{\langle \psi_{2s} | V | \psi_n \rangle \langle \psi_n | V | \psi_{1s} \rangle}{\epsilon - \epsilon_n} \quad (29)$$

$$V_{2p_m,1s}^{\text{pol}}(r_0) \equiv \sum_{\substack{\text{all } n \\ \text{except } \epsilon_n = \epsilon}} \frac{\langle \psi_{2p_m} | V | \psi_n \rangle \langle \psi_n | V | \psi_{1s} \rangle}{\epsilon - \epsilon_n}. \quad (30)$$

For large  $r_0$  these potentials have the asymptotic forms

$$V_{2s,1s}^{\text{pol}} \xrightarrow{r_0 \rightarrow \infty} -\frac{\alpha_{2s,1s}}{2r_0^4} \quad (31)$$

and

$$V_{2p_m,1s}^{\text{pol}} \xrightarrow{r_0 \rightarrow \infty} -\frac{\alpha_{2p,1s}}{2r_0^5} \delta_{m,0} \quad (32)$$

where, in the 2p case, the axis of quantisation is taken to be the direction of  $r_0$ .

For  $\epsilon = \epsilon_{1s}$  and  $\epsilon = \epsilon_{2s}$  in (29) we obtain by standard methods (Damburg and Geltman 1968)§

$$\alpha_{2s,1s} = -56\sqrt{2} \left(\frac{2}{3}\right)^6 \text{ au} \quad (33a)$$

$$\alpha_{2s,1s} = +450\sqrt{2} \left(\frac{2}{3}\right)^8 \text{ au} \quad (33b)$$

† Since only intermediate p states contribute to (27) the exact inclusion of 2s is irrelevant to the determination of  $\bar{\epsilon}$ .

‡ The zero of the energy scale is such that  $\epsilon_{1s} = -0.5$  au.

§ Our atomic hydrogen states are taken to be of the usual form  $R_{nl}(r)Y_{lm}(\theta, \phi)$  where we adopt the phase conventions of Rose (1957) for the spherical harmonics  $Y_{lm}$  and those of Bethe and Salpeter (1957) p 15 for the radial functions  $R_{nl}$ .



respectively. To reproduce these values in a closure approximation in which only the intermediate 2p state is treated exactly (in fact, the 2p state does not contribute to (33b), see (29)) requires

$$\bar{\epsilon} = 0 \text{ au} \quad (34a)$$

$$\bar{\epsilon} = -0.025 \text{ au.} \quad (34b)$$

For values of  $\epsilon$  other than  $\epsilon_{1s}$  and  $\epsilon_{2s}$  the polarisability  $\alpha_{2s,1s}$  is not so readily calculated. Not wishing to bias the choice of  $\bar{\epsilon}$  towards either the 1s state or the 2s state, a reasonable value for  $\bar{\epsilon}$  in the scattering calculation would be the average of (34a) and (34b), i.e.

$$\bar{\epsilon} = -0.0125 \text{ au.} \quad (35)$$

Similarly, for 2p we get

$$\alpha_{2p,1s} = +776 \sqrt{2} \left(\frac{2}{3}\right)^8 \quad (36a)$$

$$\alpha_{2p,1s} = -608 \sqrt{2} \left(\frac{2}{3}\right)^8 \quad (36b)$$

when  $\epsilon = \epsilon_{1s}$  and  $\epsilon_{2p}$  respectively. Again treating only the intermediate 2p contribution exactly, the closure approximation gives

$$\bar{\epsilon} = -0.0909 \text{ au} \quad (37a)$$

$$\bar{\epsilon} = -0.0658 \text{ au} \quad (37b)$$

for (36a) and (36b) respectively, with an average

$$\bar{\epsilon} = -0.0783 \text{ au.} \quad (38)$$

For the  $1s \rightarrow 2s$  and  $1s \rightarrow 2p$  excitation reactions we have used (35) and (38) respectively for our average energies in the simplified second Born approximation. However, for elastic  $1s \rightarrow 1s$  scattering we have made a more sophisticated choice than (28) for the average energy.

In the case of elastic scattering it is relatively easy to calculate the exact forward plane-wave second Born amplitude (Prasad 1964, Holt 1972):

$$f_{B2}^{PW}(\mathbf{k}_0, \mathbf{k}_0) = -\frac{1}{8\pi^4} \sum_{\text{all } n} \left( \lim_{\eta \rightarrow 0+} \int \frac{\langle \mathbf{k}_0, \psi_{1s} | V | \mathbf{k}, \psi_n \rangle \langle \mathbf{k}, \psi_n | V | \mathbf{k}_0, \psi_{1s} \rangle}{k_n^2 - k^2 + i\eta} d\mathbf{k} \right). \quad (39)$$

The imaginary part of this amplitude is obtained, via the optical theorem, from the first Born total cross section; the real part may be calculated from a dispersion relation also involving the first Born total cross section (Woolings 1972). In table 1 we give the amplitude (39) at the energies of interest to us. The possibility now arises of choosing the average energy  $\bar{\epsilon}$  so that the simplified second Born approximation to  $f_{B2}^{PW}$  correctly reproduces the exact forward values.

First, however, let us examine how sensitive the forward amplitude is to  $\bar{\epsilon}$ . Including the 1s, 2s and 2p intermediate state contributions to (39) exactly, it is found that the real part of  $f_{B2}^{PW}(\mathbf{k}_0, \mathbf{k}_0)$  is very insensitive to  $\bar{\epsilon}$  for reasonable excursions in  $\bar{\epsilon}$  about the value (28), in particular, we have checked that there is very little sensitivity in the range  $-0.1 \leq \bar{\epsilon} \leq 0.6$ . This result is not totally surprising since at asymptotically high energies the leading behaviour of  $\text{Re } f_{B2}^{PW}(\mathbf{k}_0, \mathbf{k}_0)$  is independent of  $\bar{\epsilon}$  (Byron and Joachain 1977a). It would appear that the same is true to a very good approximation at lower energies. This means that it is not a practical proposition to vary  $\bar{\epsilon}$  in order to

obtain perfect agreement with the exact values for the real part. By contrast, the imaginary part of  $f_{B2}^{PW}$  is much more sensitive to the value of  $\bar{\epsilon}$ .

In table 1 we also list the simplified second Born approximation values for  $f_{B2}^{PW}(\mathbf{k}_0, \mathbf{k}_0)$  calculated with  $\bar{\epsilon} = +0.0779$  au (see (28)). The real parts of these numbers are quite close to the exact results; the small differences between the two are significant; they are not the result of numerical inaccuracy in the calculations. The imaginary parts of the simplified second Born numbers compare favourably with the exact imaginary parts at high energies but not at low energies. To bring the two into agreement  $\bar{\epsilon}$  must be chosen according to the entries in column six of table 1.

**Table 1.** Forward second Born amplitude for elastic electron-hydrogen scattering (atomic units).

Energy (eV)	Exact real part	SSBA† real part	Exact imaginary part	SSBA† imaginary part	Average energy $\bar{\epsilon}_I$ (au) (see text)
30	2.475	2.522	1.459	1.831	0.3241
50	1.959	1.885	1.601	1.809	0.3084
100	1.350	1.283	1.513	1.592	0.2148
200	0.920	0.882	1.294	1.325	0.1575
300	0.737	0.711	1.154	1.174	0.1395
400	0.631	0.611	1.057	1.071	0.1309
500	0.560	0.543	0.984	0.996	0.1259
680	0.476	0.463	0.890	0.899	0.1207

† Simplified second Born approximation: 1s, 2s and 2p intermediate states treated exactly, contributions of remaining states approximated by closure with average energy  $\bar{\epsilon} = +0.0779$  au

In view of the above we decided to use two values of  $\bar{\epsilon}$ , one,  $\bar{\epsilon}_R$ , for the principal part of the  $k$  integration in (24), the other,  $\bar{\epsilon}_I$ , for the pole contribution to this integral‡. These two parts of the  $k$  integration in (39) lead to the real and imaginary parts of  $f_{B2}^{PW}$  respectively. For  $\bar{\epsilon}_R$  we took the value (28), for all incident energies. This, as previously described, ensures that the correct dipole polarisability of the target atom is built into the calculations; it is in  $\text{Re } f_{B2}^{PW}$ , and not  $\text{Im } f_{B2}^{PW}$ , that the dipole polarisability of the target manifests itself in the low-energy limit (see Walters 1976*b*). For  $\bar{\epsilon}_I$  we took the (energy-dependent) values listed in table 1.

In summary therefore:

(i) for elastic scattering two values of  $\bar{\epsilon}$  have been used,  $\bar{\epsilon}_R = +0.0779$  au and  $\bar{\epsilon}_I$  as given in column six of table 1;

(ii) for the 1s → 2s excitation,  $\bar{\epsilon} = -0.0125$  au;

(iii) for the 1s → 2p excitation,  $\bar{\epsilon} = -0.0783$  au.

The 2s and 2p intermediate states have always been treated exactly.

#### 4. Approximate methods for simplifying the evaluation of distorted-wave second-order amplitudes

The presence of distorted waves in the second-order terms of (15), (18) and (20) makes these amplitudes difficult to evaluate. If the distorted waves could be replaced by plane

‡ This applies, of course, only for  $n \geq N + M + 1$  in (24).

waves much computer time would be saved. It was this consideration which led Dewangan and Walters (1977) to suggest an approximation, for elastic scattering, whereby a distorted-wave second-order amplitude like that of (15) could be easily generated from the corresponding plane-wave amplitude. For electron elastic scattering by He and Ne the approximation seemed to work well.

The Dewangan-Walters approximation may be readily generalised to the case of inelastic scattering. Thus, following the same procedure as these authors we may write the second-order terms in (15), (18) and (20) as<sup>†</sup>

$$\begin{aligned}
 & -\frac{1}{2\pi} \langle F_{1s,1s}^-, \psi_{1s} | V_2 G_0^+ V_2 | F_{1s,1s}^+, \psi_{1s} \rangle \\
 & \simeq -\frac{1}{2\pi} \langle \mathbf{k}_f, \psi_{1s} | V_2 G_0^+ V_2 | \mathbf{k}_0, \psi_{1s} \rangle - \frac{2\pi i}{k_0} \sum_{J=0}^{\infty} B_{JJ}^{1s-1s} T_{JJ}^{1s-1s}(k_0; 1s) \\
 & \quad \times (1 + \frac{1}{4} T_{JJ}^{1s-1s}(k_0; 1s)) \mathcal{Y}_{00}^{J, J^0, J^0}(\hat{\mathbf{k}}_0, \hat{\mathbf{k}}_f) \quad (40a)
 \end{aligned}$$

$$\begin{aligned}
 & -\frac{1}{2\pi} \langle F_{2s,2s}^-, \psi_{2s} | V_2 G_0^+ V_2 | F_{1s,1s}^+, \psi_{1s} \rangle \\
 & \simeq -\frac{1}{2\pi} \langle \mathbf{k}_f, \psi_{2s} | V_2 G_0^+ V_2 | \mathbf{k}_0, \psi_{1s} \rangle - \frac{2\pi i}{\sqrt{k_0 k_f}} \sum_{J=0}^{\infty} B_{JJ}^{2s-1s} (\frac{1}{2} T_{JJ}^{2s-2s}(k_f; 1s+2s) \\
 & \quad + \frac{1}{2} T_{JJ}^{1s-1s}(k_0; 1s+2s) + \frac{1}{4} T_{JJ}^{2s-2s}(k_f; 1s+2s) T_{JJ}^{1s-1s}(k_0; 1s+2s)) \\
 & \quad \times \mathcal{Y}_{00}^{J, J^0, J^0}(\hat{\mathbf{k}}_0, \hat{\mathbf{k}}_f) \quad (40b)
 \end{aligned}$$

$$\begin{aligned}
 & -\frac{1}{2\pi} \sum_{\mu=-1,0,+1} \langle F_{2p_m,2p_\mu}^-, \psi_{2p_\mu} | V_2 G_0^+ V_2 | F_{1s,1s}^+, \psi_{1s} \rangle \\
 & \simeq -\frac{1}{2\pi} \langle \mathbf{k}_f, \psi_{2p_m} | V_2 G_0^+ V_2 | \mathbf{k}_0, \psi_{1s} \rangle \\
 & \quad - \frac{2\pi i}{\sqrt{k_0 k_f}} \sum_{J=0}^{\infty} \sum_{l=|J-1|}^{|J+1|} \left[ \frac{1}{2} B_{Jl}^{2p-1s} T_{JJ}^{1s-1s}(k_0; 1s+2p) \right. \\
 & \quad \left. + \frac{1}{2} \left( \sum_{l'=|J-1|}^{|J+1|} T_{Jl'}^{2p-2p}(k_f; 1s+2p) B_{Jl'}^{2p-1s} \right) (1 + \frac{1}{2} T_{JJ}^{1s-1s}(k_0; 1s+2p)) \right] \\
 & \quad \times \mathcal{Y}_{0,m}^{J, J^0, l^1}(\hat{\mathbf{k}}_0, \hat{\mathbf{k}}_f) \quad (40c)
 \end{aligned}$$

where

$$\begin{aligned}
 & -\frac{1}{2\pi} \langle \mathbf{k}_f, \psi_f | V_2 G_0^+ V_2 | \mathbf{k}_0, \psi_{1s} \rangle \\
 & = -\frac{2\pi i}{\sqrt{k_0 k_f}} \sum_{J=0}^{\infty} \sum_{l=|J-l_f|}^{|J+l_f|} B_{Jl}^{f-1s} \mathcal{Y}_{0m_f}^{J, J^0, l_f}(\hat{\mathbf{k}}_0, \hat{\mathbf{k}}_f) \quad f = 1s, 2s, 2p \quad (41a)
 \end{aligned}$$

<sup>†</sup> We refer the reader to Dewangan and Walters (1977) for the precise details of the method. Note however that, for elastic scattering, we have used a different convention for the partial-wave amplitudes from that adopted by Dewangan and Walters.

$$\begin{aligned}
& -\frac{1}{2\pi} \langle \mathbf{k}_f, \psi_f | V_1 | \Phi_i^+ (\mathbf{k}_i) \rangle \\
& = -\frac{2\pi i}{\sqrt{k_i k_f}} \sum_{J=0}^{\infty} \sum_{l=|J-l_f|}^{J+l_f} \sum_{l'=|J-l_i|}^{J+l_i} T_{Jl}^{f-i} (\mathbf{k}_i; \text{states}) \mathcal{Y}_{m_i m_f}^{J, l' l_f} (\hat{\mathbf{k}}_i, \hat{\mathbf{k}}_f)
\end{aligned} \quad (41b)$$

$$\begin{aligned}
& \mathcal{Y}_{m_i m_f}^{J, l' l_f} (\hat{\mathbf{k}}_i, \hat{\mathbf{k}}_f) \\
& \equiv \sum_{\nu=-l'}^{+l'} C(l, l_f, J, \nu + m_i - m_f, m_f) \\
& \quad \times C(l', l_i, J, \nu, m_i) Y_{l(\nu+m_i-m_f)} (\hat{\mathbf{k}}_f) Y_{l'\nu}^* (\hat{\mathbf{k}}_i)
\end{aligned} \quad (41c)$$

$l_i$  and  $l_f$  are the orbital angular momenta of the atomic states  $\psi_i$  and  $\psi_f$  respectively,  $m_i$  and  $m_f$  are the corresponding  $z$  components; 'states' in (41b) indicates the states included in the close-coupling calculation of  $\Phi_i^+$ ; the  $C$  and  $Y$  are respectively the Clebsch-Gordan coefficients and spherical harmonics of Rose (1957); \* denotes complex conjugation, and a  $\hat{\phantom{x}}$  labels a unit vector. Finally, we remark that if the wavefunctions  $F_m^\pm$  are replaced by the singlet and triplet wavefunctions  $F_m^{\pm(1),(3)}$  then the partial-wave amplitudes  $T_{Jl}^{f-i}$  must be those calculated in the appropriate close-coupling approximation with exchange.

The reader should not be put off by the notational complexities of equations (40). The results expressed are very simple. Essentially, the plane-wave approximation is to be corrected by a term which allows for scattering by  $V_1$  within the initial and final states. In the partial-wave format in which the correction terms in (40) have been cast, this amounts to taking the product of the (plane-wave) second-order amplitude,  $B_{Jl}$ , with a close-coupling amplitude  $T_{Jl'}$ , of the same total angular momentum  $J$ , appropriate to the particular initial- or final-state scattering. Two types of term arise (best seen in (40b)): the first, the product of  $B$  with a single  $T$ , represents scattering by  $V_1$  in the initial state but not in the final state, or vice versa; the second, the product of  $B$  with two  $T$ , represents scattering by  $V_1$  in both the initial and final states.

Another procedure for simplifying the calculation of distorted-wave second-order amplitudes is that used by Winters (1978, 1979). This method which has also been explored by other authors, if only in an approximate form and for elastic scattering (see, for example, Byron and Joachain 1974, 1977b), involves generating a local second-order potential from the plane-wave second Born amplitude. Thus if the distorted-wave second-order amplitude of (15) is to be calculated the local potential

$$V_{1s,1s}^{(2)}(r_0) = \frac{1}{2\pi^2 r_0} \int_0^\infty q \sin qr_0 \langle \mathbf{k}_f, \psi_{1s} | V_2 G_0^+ V_2 | \mathbf{k}_0, \psi_{1s} \rangle dq \quad (42a)$$

$$\mathbf{q} = \mathbf{k}_0 - \mathbf{k}_f \quad (42b)$$

is first computed. In analytical form (see, for example, Byron and Joachain 1973) the amplitude  $\langle \mathbf{k}_f, \psi_{1s} | V_2 G_0^+ V_2 | \mathbf{k}_0, \psi_{1s} \rangle$  is written as a function of  $k_0$ ,  $k_f (= k_0)$  and  $q$ ; hence it can easily be integrated over  $q$  from 0 to  $\infty$ , even though the *physical* second Born amplitude is only defined for  $0 \leq q \leq 2k_0$ . The distorted-wave second-order amplitude of (15) is then calculated as

$$\langle F_{1s,1s}^-, \psi_{1s} | V_2 G_0^+ V_2 | F_{1s,1s}^+, \psi_{1s} \rangle = \int F_{1s,1s}^{-*}(\mathbf{r}_0) V_{1s,1s}^{(2)}(\mathbf{r}_0) F_{1s,1s}^+(\mathbf{r}_0) d\mathbf{r}_0 \quad (43)$$

In the particular case that the functions  $F_{1s,1s}^+$  and  $F_{1s,1s}^-$  are the plane waves  $\exp(i\mathbf{k}_0 \cdot \mathbf{r}_0)$

and  $\exp(ik_f \cdot r_0)$  respectively, the approximation (43) is exact. To evaluate (18) one defines, in a similar fashion to (42) and (43), a local second-order potential  $V_{2s,1s}^{(2)}$  (Winters 1978). So far, the local potential approach has only been used for s-s transitions.

Although the local potential method has appeared in several papers (Winters 1978, 1979, Vanderpoorten and Winters 1978, 1979) its viability seems to have been tested only for the elastic scattering of electrons by helium (Bransden *et al* 1978)—a test which it passed well. In the present work we compare the local potential approximation with exact results for the inelastic scattering  $1s \rightarrow 2s$ ; we also re-check the validity of the method for elastic scattering, this time the elastic scattering of electrons by hydrogen.

These tests have been made possible by our 'exact' calculation of the distorted-wave second-order amplitudes in (15), (18) and (20) at a number of energies. By 'exact' we here mean that the *only* approximation we have made in evaluating the second-order amplitudes is the Holt-Moiseiwitsch simplified second Born approximation to the sum over intermediate target states (see § 3). Thus we have not resorted to any kind of further approximation, such as making an 'on-energy-shell' assumption (Dewangan and Walters) or localising the potential  $V_2 G_0^+ V_2$  (Winters), in handling the distorted-wave part of the calculation, i.e. distortion effects have been calculated *exactly*. The 'exact' calculations involve a numerical procedure based upon partial-wave analysis. The method is similar to, although by no means identical with, that used by Winters *et al* (1974) in the second-order potential model.

## 5. Results

### 5.1. Elastic scattering

*5.1.1. Comments on the calculations and the approximate methods for simplifying the evaluation of distorted-wave second-order amplitudes.* The second-order amplitude in (15) has been calculated with *exact*<sup>†</sup> allowance for distortion at 30, 50, 100 and 200 eV and the results have been compared with those of the approximate methods of § 4.

At 100 eV the Dewangan-Walters prescription (40a) gives a DWSBA differential cross section different from the *exact*<sup>†</sup> values by at most 3%<sup>‡</sup> at any angle; at 0° the deviation is as small as 1%. This is a triumph for the approximation since the difference between using distorted waves and plane waves in (15) is a change in the elastic cross section varying from 6% at 0° to 37% at 180°. On going to 200 eV the Dewangan-Walters approximation gets better, but correspondingly deteriorates towards lower energies: at 50 eV the maximum deviation from the exact cross section is 7%; while at 30 eV the difference ranges from 5% at 0° to a maximum of 30% at 180°.

The viability of the Dewangan-Walters approximation at the higher energies vindicates its previous use in elastic  $e^-$ -Ne scattering (Dewangan and Walters 1977), where the lowest energy studied was 100 eV. In fact, we have also calculated the *exact*<sup>†</sup> DWSBA cross section for He at 100 eV and found agreement, within 5% at any angle, with the former work. Dewangan and Walters (1977) also applied their prescription to elastic  $e^-$ -Ne scattering. While it would be rash to conclude that their approximation also works well for Ne, there is too big a difference between He and Ne, e.g. Ne has a much stronger static field than He, we may be optimistic.

<sup>†</sup> See last paragraph of § 4.

<sup>‡</sup> Quoted percentages are relative to the exact DWSBA values.

Now let us turn to the approximate method used by Winters. We have calculated the DWSBA cross sections at 30 and 50 eV using the local second-order potential (42). The agreement obtained with the exact<sup>†</sup> DWSBA was very good: at 30 eV the maximum difference was around 4%; at 50 eV around 3%. This confirms the results obtained with He (Bransden *et al* 1978). The Winters approximation is clearly a very accurate one, better than the Dewangan–Walters prescription in that it remains viable to lower energies. Again it is an open question whether the Winters method would be as valid for a heavier atom, like Ne.

Finally, we inform the reader that the DWSBA elastic cross sections at 30, 50, 100 and 200 eV reported in this paper have been calculated with exact<sup>†</sup> allowance for distortion in the second-order amplitude of (15); those at 300, 400 and 680 eV have been obtained using the Dewangan–Walters approximation (40a).

*5.1.2. Differential cross sections.* In the energy range of interest to us, i.e. 30 eV upwards, there are three sets of experimental cross sections: Lloyd *et al* (1974), Williams (1975) and van Wingerden *et al* (1977).

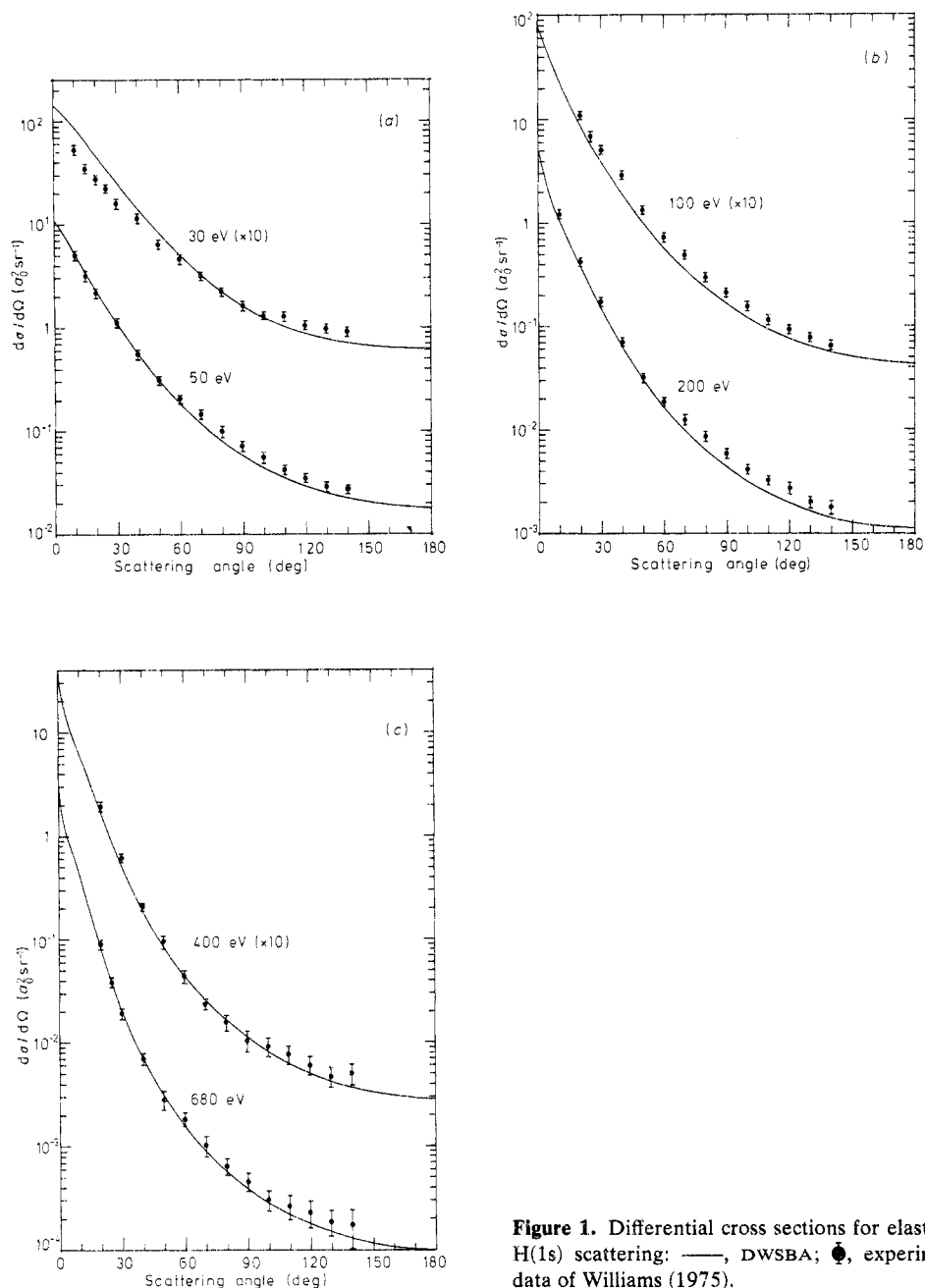
Lloyd *et al* measured ratios of  $e^-$ -H to  $e^-$ -H<sub>2</sub> elastic scattering; by adopting suitable values for the molecular cross sections the atomic cross sections were then placed on an absolute scale, but with an estimated normalisation error as high as 40%. Later van Wingerden *et al* (1977), while making an absolute determination of the  $e^-$ -H<sub>2</sub> elastic differential cross section, decided to use their measurements together with the cross section ratios of Lloyd *et al* to produce absolute atomic hydrogen cross sections at 100 and 200 eV, this time with an estimated accuracy of around 10%. However, van Wingerden *et al* remarked upon a seeming inconsistency in their results: at small momentum transfers the 100 eV cross sections were not noticeably higher than the corresponding 200 eV values, contrary to expectation.

In view of the above, and for the sake of clarity, we have thought it best to make a graphical comparison only with the data of Williams (1975). These data have quoted errors of around 10% and cover a wider energy range, 30 to 680 eV, than the measurements of Lloyd *et al* and van Wingerden *et al*. We compare our DWSBA cross sections with the Williams data in figure 1.

At 50 eV and above, but with the exception of 100 eV, the agreement between the DWSBA and experiment is fairly good. At 50 and 200 eV we note that the DWSBA underestimates the experimental cross section in the angular region beyond about 60°. This same pattern of discrepancy can also be discerned in the work of Dewangan and Walters (1977) on He and in precisely the same angular range. Another feature which also agrees with the work of these authors on He and Ne, is the mode of breakdown of the DWSBA at low energies. From figure 1 we see that breakdown sets in rapidly between 50 and 30 eV; at 30 eV the DWSBA in the forward angular region greatly exceeds the experimental cross section—exactly as in He and Ne! Ermolaev and Walters (1979) have suggested that the primary cause of this breakdown may be the neglect of second-order, and perhaps higher order, exchange effects other than those arising in the static exchange approximation.

We turn now to the disagreement between the DWSBA and the data of Williams (1975) at 100 eV. Here the theoretical cross section is always smaller than the measured values. It is interesting to see what light is thrown upon this situation by the 100 eV results of van Wingerden *et al* (1977). This latter cross section lies nearly

<sup>†</sup> See last paragraph of § 4.



**Figure 1.** Differential cross sections for elastic  $e^-$ -H(1s) scattering: —, DWSBA;  $\bullet$ , experimental data of Williams (1975).

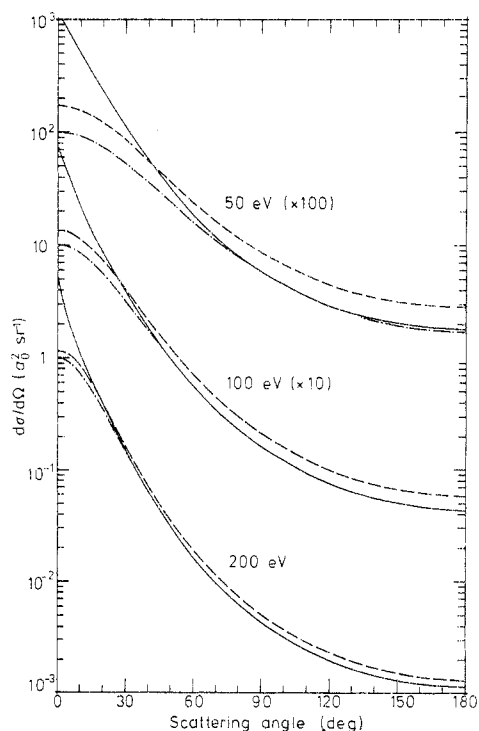
everywhere above that of Williams, exceeding his values, on average, by a factor of 1.05; van Wingerden *et al* clearly favour Williams data rather than the DWSBA. However, we have seen above that, consistent with the patterns observed in He and Ne, the breakdown mode of the DWSBA seems to be to give too large a cross section in the forward angular region. Yet at 100 eV the DWSBA cross section lies *below* the experimental data. Furthermore, at the two energies on either side of 100 eV, i.e. 50

and 200 eV, the DWSBA is in quite good agreement with the measurements. These last two considerations lead us to suggest, with reasonable certainty, that the measurements of Williams at 100 eV are in error; our certainty is not shaken by the support lent to the Williams data by the results of van Wingerden *et al*; we saw earlier that the 100 and 200 eV cross sections of van Wingerden *et al* do not seem to be consistent with one another.

In figure 2 we compare the DWSBA numbers with the first Born approximation (FBA) at 50, 100 and 200 eV. A surprising situation is revealed, the close agreement between the FBA and DWSBA at large angles. On the scale of figure 2 the FBA cross sections are indistinguishable from the DWSBA values for angles between 80 and 130° at 50 eV, and for angles greater than about 50° and 30° at 100 and 200 eV respectively; by 680 eV the FBA cross section only differs significantly from the DWSBA at angles less than about 7°. This rapid convergence of the DWSBA to the FBA arises in a non-trivial fashion. We can illustrate this point by considering the pure static exchange cross sections; these are also shown in figure 2. The static exchange approximation still differs noticeably from the DWSBA at those angles where the FBA and DWSBA agree. Since the static exchange amplitude is part of the DWSBA amplitude (see (15)) the rapid convergence of the DWSBA to the FBA must be the result of cancellations within the DWSBA.

Finally, we remark upon the similarity of our DWSBA results to those obtained by Byron and Joachain (1977a) and Winters *et al* (1974) in the eikonal Born series approximation and second-order potential method respectively. The relationship between the three approximations has been discussed by Dewangan and Walters (1977).

Our DWSBA elastic differential cross sections are given in table 2.



**Figure 2.** Comparison of DWSBA, FBA and static exchange differential cross sections for elastic  $e^-$ -H(1s) scattering: —, DWSBA; ---, static exchange; - · - · -, FBA.



**Table 2.** DWSBA differential cross sections (in units of  $a_0^2 \text{ sr}^{-1}$ ) for elastic  $1s \rightarrow 1s$  scattering of electrons by atomic hydrogen.

Angle (deg)	Energy (eV)							
	30	50	100	200	300	400	500	680
0	0.142 <sup>2†</sup>	0.108 <sup>2</sup>	0.749 <sup>1</sup>	0.520 <sup>1</sup>	0.423 <sup>1</sup>	0.369 <sup>1</sup>	0.333 <sup>1</sup>	0.292 <sup>1</sup>
2	0.130 <sup>2</sup>	0.953 <sup>1</sup>	0.598 <sup>1</sup>	0.348 <sup>1</sup>	0.246 <sup>1</sup>	0.195 <sup>1</sup>	0.166 <sup>1</sup>	0.137 <sup>1</sup>
4	0.119 <sup>2</sup>	0.825 <sup>1</sup>	0.462 <sup>1</sup>	0.235 <sup>1</sup>	0.162 <sup>1</sup>	0.131 <sup>1</sup>	0.115 <sup>1</sup>	0.985
6	0.107 <sup>2</sup>	0.706 <sup>1</sup>	0.357 <sup>1</sup>	0.171 <sup>1</sup>	0.121 <sup>1</sup>	0.996	0.878	0.748
8	0.961 <sup>1</sup>	0.600 <sup>1</sup>	0.279 <sup>1</sup>	0.132 <sup>1</sup>	0.945	0.781	0.679	0.558
10	0.858 <sup>1</sup>	0.509 <sup>1</sup>	0.222 <sup>1</sup>	0.105 <sup>1</sup>	0.754	0.613	0.520	0.407
14	0.678 <sup>1</sup>	0.366 <sup>1</sup>	0.146 <sup>1</sup>	0.694	0.483	0.370	0.295	0.209
20	0.530 <sup>1</sup>	0.226 <sup>1</sup>	0.848	0.386	0.243	0.169	0.125	0.785 <sup>-1</sup>
25	0.469 <sup>1</sup>	0.155 <sup>1</sup>	0.564	0.238	0.139	0.907 <sup>-1</sup>	0.637 <sup>-1</sup>	0.379 <sup>-1</sup>
30	0.344 <sup>1</sup>	0.108 <sup>1</sup>	0.383	0.150	0.816 <sup>-1</sup>	0.510 <sup>-1</sup>	0.347 <sup>-1</sup>	0.200 <sup>-1</sup>
35	0.253 <sup>1</sup>	0.770	0.266	0.960	0.500 <sup>-1</sup>	0.303 <sup>-1</sup>	0.203 <sup>-1</sup>	0.114 <sup>-1</sup>
40	0.141 <sup>1</sup>	0.557	0.187	0.635 <sup>-1</sup>	0.320 <sup>-1</sup>	0.190 <sup>-1</sup>	0.125 <sup>-1</sup>	0.698 <sup>-2</sup>
50	0.814	0.308	0.985 <sup>-1</sup>	0.305 <sup>-1</sup>	0.147 <sup>-1</sup>	0.855 <sup>-2</sup>	0.556 <sup>-2</sup>	0.306 <sup>-2</sup>
60	0.495	0.182	0.562 <sup>-1</sup>	0.165 <sup>-1</sup>	0.776 <sup>-2</sup>	0.446 <sup>-2</sup>	0.288 <sup>-2</sup>	0.157 <sup>-2</sup>
75	0.262	0.948 <sup>-1</sup>	0.281 <sup>-1</sup>	0.778 <sup>-2</sup>	0.361 <sup>-2</sup>	0.205 <sup>-2</sup>	0.132 <sup>-2</sup>	0.720 <sup>-3</sup>
90	0.160	0.572 <sup>-1</sup>	0.162 <sup>-1</sup>	0.435 <sup>-2</sup>	0.200 <sup>-2</sup>	0.113 <sup>-2</sup>	0.730 <sup>-3</sup>	0.397 <sup>-3</sup>
110	0.102	0.350 <sup>-1</sup>	0.932 <sup>-2</sup>	0.245 <sup>-2</sup>	0.112 <sup>-2</sup>	0.632 <sup>-3</sup>	0.406 <sup>-3</sup>	0.221 <sup>-3</sup>
120	0.879 <sup>-1</sup>	0.292 <sup>-1</sup>	0.756 <sup>-2</sup>	0.197 <sup>-2</sup>	0.894 <sup>-3</sup>	0.506 <sup>-3</sup>	0.325 <sup>-3</sup>	0.177 <sup>-3</sup>
140	0.713 <sup>-1</sup>	0.223 <sup>-1</sup>	0.556 <sup>-2</sup>	0.140 <sup>-2</sup>	0.646 <sup>-3</sup>	0.366 <sup>-3</sup>	0.235 <sup>-3</sup>	0.127 <sup>-3</sup>
160	0.641 <sup>-1</sup>	0.191 <sup>-1</sup>	0.462 <sup>-2</sup>	0.118 <sup>-2</sup>	0.536 <sup>-3</sup>	0.303 <sup>-3</sup>	0.195 <sup>-3</sup>	0.106 <sup>-3</sup>
180	0.621 <sup>-1</sup>	0.181 <sup>-1</sup>	0.433 <sup>-2</sup>	0.113 <sup>-2</sup>	0.504 <sup>-3</sup>	0.285 <sup>-3</sup>	0.183 <sup>-3</sup>	0.994 <sup>-4</sup>

† The superscripts to the numbers denote the power of 10 by which they should be multiplied.

**5.1.3. Total elastic cross sections.** Some of the differential cross sections of Williams (1975) have been extrapolated and integrated by de Heer *et al* (1977) to give total elastic cross sections. These cross sections are presented in table 3 together with those obtained in the DWSBA, static exchange approximation and FBA. Consistent with the differential cross section comparisons the DWSBA results agree well with the experimental values at 50 and 200 eV but are a lot smaller at 100 eV.

**Table 3.** Total cross sections for elastic  $1s \rightarrow 1s$  scattering of electrons by atomic hydrogen (in units of  $\pi a_0^2$ ).

Energy (eV)	Experimental values Williams (1975)†	DWSBA	Pure static exchange	First Born
30		2.674	1.691	0.868
50	1.24	1.223	0.886	0.563
100	0.588	0.463	0.383	0.299
200	0.204	0.194	0.175	0.154
300		0.121	0.113	0.104
400	0.0653	0.088	0.083	0.078
500		0.069	0.066	0.063
680		0.050	0.048	0.046

† As given by de Heer *et al* (1977).

The experimental cross section at 400 eV is curious; it is much smaller than both the DWSBA and FBA. Yet, from figure 1(c) we see that, if anything, the experimental data of Williams lie slightly higher than the DWSBA. To calculate the integrated experimental cross section the data of Williams have to be extrapolated from 20 to 0°. Since the FBA is in good agreement with the DWSBA at angles above 20°, and since the FBA lacks a forward 'polarisation peak', any sensible extrapolation to 0° would have to give a cross section not lying below the FBA in the angular region 0 to 20°. We conclude that the integrated experimental cross section should not lie below the FBA value. Since the 400 eV experimental cross section of table 3 violates this lower bound, we suggest that it is in error.

We see from table 3 that there is still a marked difference between the DWSBA and FBA even at an energy as high as 680 eV, this despite the agreement between the two differential cross sections for angles greater than 7° (see § 5.1.2). The difference in integrated cross sections arises from the sharp forward 'polarisation peak' in the DWSBA differential cross section which is not possessed by the FBA.

The static exchange cross sections are in better agreement with the DWSBA than those of the FBA. The reason should be clear from figure 2.

**5.1.4. Total cross sections.** We have calculated the electron-hydrogen total scattering cross section by applying the optical theorem to the imaginary parts of the forward DWSBA (singlet and triplet) amplitudes. Our results are given in table 4 together with the semi-empirical estimates of de Heer *et al* (1977); these latter cross sections are considered to have an accuracy of 10%. At 100 eV and above there is agreement between the two sets of numbers within the 10% error; at the higher energies this agreement is particularly good. Below 100 eV the DWSBA cross section becomes larger than the semi-empirical values. This is a breakdown pattern of the DWSBA which has also been observed in the cases of He and Ne (Dewangan and Walters 1977).

This last remark requires further comment. The average closure energy  $\bar{\epsilon}$  used in the work of Dewangan and Walters on He and Ne was chosen in the same way as that used to calculate the numbers in column five of table 1. Comparing columns four and five of table 1 we see that a substantial error results in the (plane-wave) simplified second Born amplitude at low energies. The nature of this error is such that the corresponding total cross section would be too large. A significant part of the error in the DWSBA total cross sections for He and Ne probably therefore arises from the choice of  $\bar{\epsilon}$ . That this is not the only substantial source of error, however, is shown by the

**Table 4.** Total cross sections for the scattering of electrons by atomic hydrogen (in units of  $\pi a_0^2$ ).

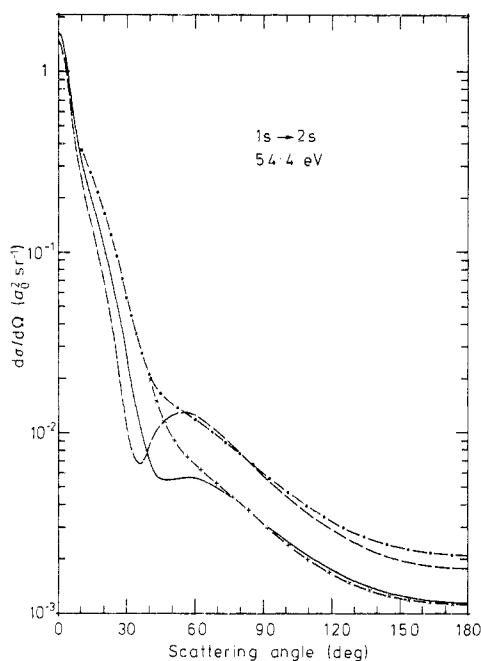
Energy (eV)	DWSBA	Semi-empirical de Heer <i>et al</i> (1977)
30	5.131	4.05
50	3.790	3.28
100	2.354	2.18
200	1.383	1.33
300	0.991	0.975
400	0.784	0.775
500	0.653	
680	0.505	

present work: the DWSBA cross section of table 4 has been calculated in a closure approximation which gives an accurate forward (plane-wave) second Born amplitude, yet it is still too large at the lower energies.

## 5.2. Excitation of the $n = 2$ states

**5.2.1. Comments on the calculations and the approximate methods for simplifying the evaluation of distorted-wave second-order amplitudes.** We have calculated the DWSBA cross section for the  $1s \rightarrow 2s$  transition at  $54.4$  ( $k_0 = 2$  au), 100, 200 and 300 eV and for the  $1s \rightarrow 2p$  transition at  $54.4$ , 100 and 200 eV making *exact*<sup>†</sup> allowance for distortion in the second-order amplitudes of (18) and (20).

We have also calculated the DWSBA cross section for both the  $1s \rightarrow 2s$  and  $1s \rightarrow 2p$  excitations at all energies employing the prescription of Dewangan and Walters (1977) (equations (40*b*) and (40*c*)). In figure 3 we compare the result for the  $1s \rightarrow 2s$  transition at  $54.4$  eV with the *exact*<sup>†</sup> DWSBA cross section. The failure of the Dewangan–Walters prescription is clear.



**Figure 3.** Differential cross sections for  $e^- + H(1s) \rightarrow e^- + H(2s)$  at  $54.4$  eV ( $k_0 = 2$  au). —, exact DWSBA; - · -, DWSBA using Dewangan–Walters prescription (40*b*); - · · -, DWSBA using local second-order potential method of Winters; - - -, ECSSBA.

How well does the local second-order potential method of Winters fare? We also exhibit the DWSBA cross section calculated in this approximation in figure 3. Again there is general disagreement with the *exact*<sup>†</sup> numbers. Indeed, between  $0$  and  $40^\circ$  the Winters cross section agrees with the Dewangan–Walters values within about 10%. However, at large scattering angles ( $\geq 70^\circ$ ) the Winters cross section, unlike the Dewangan–Walters results, comes into agreement with the exact DWSBA.

The performances of the Dewangan–Walters prescription and of the Winters local potential method do not improve with increasing energy. We have been able to test

<sup>†</sup> See last paragraph of § 4.

both approximations for the  $1s \rightarrow 2s$  excitation up to an energy of 300 eV. With increasing energy all four curves of figure 3 approach closer to one another, reflecting the lesser importance of using distorted waves rather than plane waves<sup>†</sup> in the second-order amplitude of (18) at the higher energies, but the error in the Winters method at angles less than  $70^\circ$ , and in the Dewangan-Walters prescription at all angles, still generally remains comparable with or greater than the size of the distortion effect that the approximation is supposed to represent. The agreement between the Winters approximation and the exact<sup>‡</sup> results at angles beyond  $70^\circ$  (see figure 3) does, however, persist to the higher energies.

We have also examined the Dewangan-Walters formula (40c) against the exact<sup>‡</sup> DWSBA numbers for the  $1s \rightarrow 2p$  transition in the energy range 54.4 to 200 eV and find, as expected, that it fails once more. In view of the unreliability of the Winters method for the  $1s \rightarrow 2s$  transition we have not considered it worthwhile to generalise his procedure to the  $1s \rightarrow 2p$  case.

Why do the approximations of Dewangan and Walters and of Winters work for elastic scattering but not for inelastic scattering? We are unable at this moment to detail the precise mechanism of the success or failure of these methods; we leave this investigation to a future date. We shall be content with making the trivial observation that there is a symmetry between the initial and final states in elastic scattering which is absent for inelastic scattering.

Our present methods for including distortion exactly in the second-order amplitudes of the DWSBA are a little tedious. It is for this reason that we have calculated the exact<sup>‡</sup> DWSBA cross section only for energies up to 300 and 200 eV for  $1s \rightarrow 2s$  and  $1s \rightarrow 2p$  respectively. Comparison of the exact DWSBA results at the higher energies with the Dewangan-Walters prescription, the ECSSBA and the pure second Born approximation revealed certain regularities. These regularities suggested prescriptive procedures whereby a cross section close to the exact DWSBA values could be generated from the three cross sections mentioned above. Thus, for example, figure 3 suggests that in the angular region  $0$  to  $20^\circ$  a fair approximation to the exact DWSBA cross section might be obtained by taking one half of the sum of the Dewangan-Walters cross section and the ECSSBA<sup>§</sup>. Although we have used figure 3 to illustrate our point it is in itself a bad example; our prescriptions are designed for higher energies where, in tests against the higher energy exact DWSBA cross sections, they work very well. For brevity, we do not detail the prescriptive procedures here.

The DWSBA cross sections reported in this paper for the  $1s \rightarrow 2s$  transition at energies of 400 eV and above, and for the  $1s \rightarrow 2p$  excitation at energies of 300 eV and above, have been constructed as indicated in the previous paragraph. We estimate that the constructed  $1s \rightarrow 2s$  DWSBA cross sections represent the exact<sup>‡</sup> DWSBA values to within 2% in the angular range  $0$ – $35^\circ$  and within 5% at higher angles; the constructed  $1s \rightarrow 2p$  DWSBA cross sections are accurate to within 1%, 4% and about 10% in the angular regions  $0$ – $25^\circ$ ,  $25$ – $50^\circ$  and  $50$ – $180^\circ$  respectively.

**5.2.2. Differential cross sections.** Our DWSBA differential cross sections for the  $1s \rightarrow 2s$  and  $1s \rightarrow 2p$  transitions are given in tables 5 and 6.

<sup>†</sup> The fourth curve in figure 3 is the ECSSBA of Buckley and Walters (1975). This approximation uses plane waves in the second-order amplitude of (18).

<sup>‡</sup> See last paragraph of § 4.

<sup>§</sup> Note that the prescriptive procedures actually used vary with the angular region being considered.

**Table 5.** DWSBA differential cross sections (in units of  $a_0^2 \text{ sr}^{-1}$ ) for  $1s \rightarrow 2s$  excitation of atomic hydrogen by electron impact.

Angle (deg)	Energy (eV)						
	54.4	100	200	300	400	500	680
0	0.163 <sup>†</sup>	0.148 <sup>†</sup>	0.132 <sup>†</sup>	0.124 <sup>†</sup>	0.119 <sup>†</sup>	0.116 <sup>†</sup>	0.112 <sup>†</sup>
2	0.143 <sup>†</sup>	0.114 <sup>†</sup>	0.944	0.917	0.909	0.889	0.850
4	0.103 <sup>†</sup>	0.769	0.732	0.694	0.652	0.599	0.515
6	0.681	0.582	0.555	0.478	0.409	0.343	0.252
8	0.460	0.464	0.397	0.300	0.229	0.172	0.105
10	0.333	0.368	0.267	0.174	0.117	0.781 <sup>-1</sup>	0.403 <sup>-1</sup>
12	0.257	0.284	0.170	0.952 <sup>-1</sup>	0.559 <sup>-1</sup>	0.337 <sup>-1</sup>	0.150 <sup>-1</sup>
14	0.207	0.213	0.104	0.500 <sup>-1</sup>	0.261 <sup>-1</sup>	0.144 <sup>-1</sup>	0.579 <sup>-2</sup>
16	0.169	0.154	0.613 <sup>-1</sup>	0.258 <sup>-1</sup>	0.123 <sup>-1</sup>	0.641 <sup>-2</sup>	0.244 <sup>-2</sup>
18	0.137	0.109	0.354 <sup>-1</sup>	0.134 <sup>-1</sup>	0.604 <sup>-2</sup>	0.309 <sup>-2</sup>	0.119 <sup>-2</sup>
20	0.110	0.746 <sup>-1</sup>	0.204 <sup>-1</sup>	0.720 <sup>-1</sup>	0.324 <sup>-2</sup>	0.168 <sup>-2</sup>	0.676 <sup>-3</sup>
25	0.576 <sup>-1</sup>	0.271 <sup>-1</sup>	0.588 <sup>-2</sup>	0.215 <sup>-2</sup>	0.103 <sup>-2</sup>	0.581 <sup>-3</sup>	0.256 <sup>-3</sup>
30	0.270 <sup>-1</sup>	0.103 <sup>-1</sup>	0.259 <sup>-2</sup>	0.106 <sup>-2</sup>	0.532 <sup>-3</sup>	0.302 <sup>-3</sup>	0.131 <sup>-3</sup>
35	0.124 <sup>-1</sup>	0.522 <sup>-2</sup>	0.160 <sup>-2</sup>	0.646 <sup>-3</sup>	0.317 <sup>-3</sup>	0.175 <sup>-3</sup>	0.736 <sup>-4</sup>
40	0.690 <sup>-2</sup>	0.376 <sup>-2</sup>	0.114 <sup>-2</sup>	0.434 <sup>-3</sup>	0.20 <sup>-3</sup>	0.11 <sup>-3</sup>	0.44 <sup>-4</sup>
45	0.553 <sup>-2</sup>	0.318 <sup>-2</sup>	0.842 <sup>-3</sup>	0.302 <sup>-3</sup>	0.14 <sup>-3</sup>	0.71 <sup>-4</sup>	0.29 <sup>-4</sup>
50	0.551 <sup>-2</sup>	0.275 <sup>-2</sup>	0.611 <sup>-3</sup>	0.206 <sup>-3</sup>	0.93 <sup>-4</sup>	0.48 <sup>-4</sup>	0.19 <sup>-4</sup>
60	0.563 <sup>-2</sup>	0.195 <sup>-2</sup>	0.343 <sup>-3</sup>	0.110 <sup>-3</sup>	0.48 <sup>-4</sup>	0.24 <sup>-4</sup>	0.96 <sup>-5</sup>
75	0.450 <sup>-2</sup>	0.109 <sup>-2</sup>	0.160 <sup>-3</sup>	0.491 <sup>-4</sup>	0.21 <sup>-4</sup>	0.11 <sup>-4</sup>	0.42 <sup>-5</sup>
90	0.317 <sup>-2</sup>	0.638 <sup>-3</sup>	0.883 <sup>-4</sup>	0.267 <sup>-4</sup>	0.11 <sup>-4</sup>	0.57 <sup>-5</sup>	0.22 <sup>-5</sup>
110	0.205 <sup>-2</sup>	0.364 <sup>-3</sup>	0.488 <sup>-4</sup>	0.146 <sup>-4</sup>	0.61 <sup>-4</sup>	0.32 <sup>-5</sup>	0.13 <sup>-5</sup>
120	0.172 <sup>-2</sup>	0.293 <sup>-3</sup>	0.392 <sup>-4</sup>	0.121 <sup>-4</sup>	0.47 <sup>-4</sup>	0.25 <sup>-5</sup>	0.10 <sup>-5</sup>
140	0.135 <sup>-2</sup>	0.215 <sup>-3</sup>	0.281 <sup>-4</sup>	0.87 <sup>-5</sup>	0.34 <sup>-5</sup>	0.18 <sup>-5</sup>	0.65 <sup>-6</sup>
160	0.118 <sup>-2</sup>	0.177 <sup>-3</sup>	0.229 <sup>-4</sup>	0.72 <sup>-5</sup>	0.27 <sup>-5</sup>	0.14 <sup>-5</sup>	—
180	0.115 <sup>-2</sup>	0.17 <sup>-3</sup>	0.22 <sup>-4</sup>	—	—	—	—

† The superscripts to the numbers denote the power of 10 by which they should be multiplied.

It is of interest to compare the  $1s \rightarrow 2s$  DWSBA cross section with the ECSSBA cross section of Buckley and Walters (1975) for the  $1^1S \rightarrow 2^1S$  transition in He. In the calculations on He the ECSSBA was found to develop a pronounced dip-bump structure at the lower energies, the dip appearing at around  $30^\circ$ . The experiments also showed structure but less pronounced and appearing at a larger angle. In the angular range prior to the dip the ECSSBA tended to be lower than the experimental data, while beyond the dip (i.e. at larger angles) the ECSSBA was too large. In figure 3 we have shown both the ECSSBA and DWSBA cross sections for the  $1s \rightarrow 2s$  transition in hydrogen at 54.4 eV. We see that in going from the ECSSBA cross section to the DWSBA cross section the changes are all in the right direction: structure at intermediate angles ( $\sim 40$ – $60^\circ$ ), but less pronounced and at larger angles than in the ECSSBA; a larger cross section in the angular range leading up to the dip in the ECSSBA; a smaller cross section at large angles. We expect that the DWSBA will work well for the  $1^1S \rightarrow 2^1S$  transition in He.

Another feature highlighted by Buckley and Walters in their work on the  $1^1S \rightarrow 2^1S$  transition in He was the partial cancellation of the  $2^1P$  contribution to the second Born amplitude by other intermediate states. A consequence of this effect is that models not making sufficient allowance for this cancellation, e.g. a  $1^1S$ – $2^1S$ – $2^1P$  close-coupling calculation, give too large a cross section in the forward angular region. We might

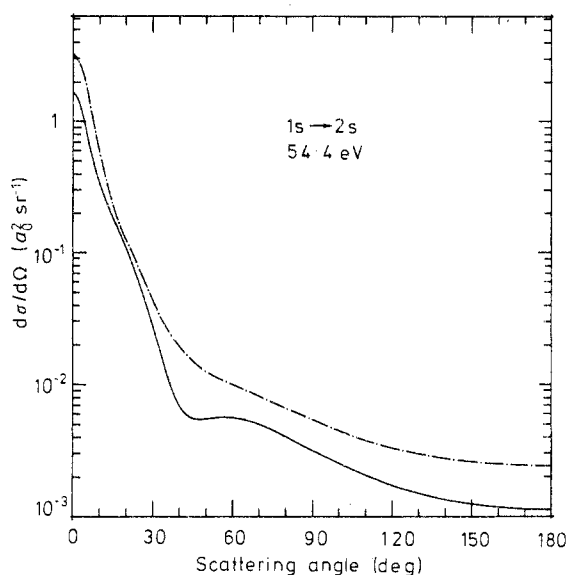
**Table 6.** DWSBA differential cross sections (in units of  $a_0^2 \text{ sr}^{-1}$ ) for  $1s \rightarrow 2p$  excitation of atomic hydrogen by electron impact.

Angle (deg)	Energy (eV)						
	54.4	100	200	300	400	500	680
0	0.463 <sup>2†</sup>	0.986 <sup>2</sup>	0.215 <sup>3</sup>	0.330 <sup>3</sup>	0.445 <sup>3</sup>	0.559 <sup>3</sup>	0.766 <sup>3</sup>
2	0.410 <sup>2</sup>	0.676 <sup>2</sup>	0.735 <sup>2</sup>	0.605 <sup>2</sup>	0.487 <sup>2</sup>	0.399 <sup>2</sup>	0.293 <sup>2</sup>
4	0.301 <sup>2</sup>	0.332 <sup>2</sup>	0.217 <sup>2</sup>	0.143 <sup>2</sup>	0.101 <sup>2</sup>	0.752 <sup>1</sup>	0.479 <sup>1</sup>
6	0.203 <sup>2</sup>	0.164 <sup>2</sup>	0.817 <sup>1</sup>	0.467 <sup>1</sup>	0.294 <sup>1</sup>	0.197 <sup>1</sup>	0.106 <sup>1</sup>
8	0.132 <sup>2</sup>	0.857 <sup>1</sup>	0.342 <sup>1</sup>	0.168 <sup>1</sup>	0.933	0.557	0.249
10	0.857 <sup>1</sup>	0.463 <sup>1</sup>	0.149 <sup>1</sup>	0.627	0.302	0.160	0.594 <sup>-1</sup>
12	0.556 <sup>1</sup>	0.255 <sup>1</sup>	0.661	0.235	0.986 <sup>-1</sup>	0.463 <sup>-1</sup>	0.146 <sup>-1</sup>
14	0.361 <sup>1</sup>	0.141 <sup>1</sup>	0.293	0.884 <sup>-1</sup>	0.327 <sup>-1</sup>	0.139 <sup>-1</sup>	0.385 <sup>-2</sup>
16	0.234 <sup>1</sup>	0.775	0.129	0.336 <sup>-1</sup>	0.113 <sup>-1</sup>	0.455 <sup>-2</sup>	0.123 <sup>-2</sup>
18	0.151 <sup>1</sup>	0.424	0.573 <sup>-1</sup>	0.131 <sup>-1</sup>	0.419 <sup>-2</sup>	0.169 <sup>-2</sup>	0.506 <sup>-3</sup>
20	0.964	0.231	0.258 <sup>-1</sup>	0.542 <sup>-2</sup>	0.173 <sup>-2</sup>	0.726 <sup>-3</sup>	0.234 <sup>-3</sup>
25	0.306	0.506 <sup>-1</sup>	0.451 <sup>-2</sup>	0.106 <sup>-2</sup>	0.399 <sup>-3</sup>	0.194 <sup>-3</sup>	0.78 <sup>-4</sup>
30	0.969 <sup>-1</sup>	0.135 <sup>-1</sup>	0.156 <sup>-2</sup>	0.482 <sup>-3</sup>	0.204 <sup>-3</sup>	0.106 <sup>-3</sup>	0.44 <sup>-4</sup>
35	0.361 <sup>-1</sup>	0.605 <sup>-2</sup>	0.916 <sup>-3</sup>	0.27 <sup>-3</sup>	0.11 <sup>-3</sup>	0.56 <sup>-4</sup>	0.22 <sup>-4</sup>
40	0.198 <sup>-1</sup>	0.412 <sup>-2</sup>	0.599 <sup>-3</sup>	0.18 <sup>-3</sup>	0.76 <sup>-4</sup>	0.39 <sup>-4</sup>	0.16 <sup>-4</sup>
45	0.150 <sup>-1</sup>	0.314 <sup>-2</sup>	0.441 <sup>-3</sup>	0.13 <sup>-3</sup>	0.53 <sup>-4</sup>	0.26 <sup>-4</sup>	0.13 <sup>-4</sup>
50	0.124 <sup>-1</sup>	0.239 <sup>-2</sup>	0.329 <sup>-3</sup>	0.98 <sup>-4</sup>	0.41 <sup>-4</sup>	0.22 <sup>-4</sup>	0.96 <sup>-5</sup>
60	0.818 <sup>-2</sup>	0.141 <sup>-2</sup>	0.196 <sup>-3</sup>	0.58 <sup>-4</sup>	0.24 <sup>-4</sup>	0.12 <sup>-4</sup>	0.58 <sup>-5</sup>
75	0.422 <sup>-2</sup>	0.706 <sup>-3</sup>	0.103 <sup>-3</sup>	0.36 <sup>-4</sup>	0.16 <sup>-4</sup>	0.86 <sup>-4</sup>	0.34 <sup>-5</sup>
90	0.271 <sup>-2</sup>	0.488 <sup>-3</sup>	0.72 <sup>-4</sup>	0.24 <sup>-4</sup>	0.11 <sup>-4</sup>	0.59 <sup>-5</sup>	0.24 <sup>-5</sup>
110	0.206 <sup>-2</sup>	0.407 <sup>-3</sup>	0.57 <sup>-4</sup>	0.18 <sup>-4</sup>	0.79 <sup>-5</sup>	0.41 <sup>-5</sup>	0.17 <sup>-5</sup>
120	0.190 <sup>-2</sup>	0.39 <sup>-3</sup>	0.51 <sup>-4</sup>	0.16 <sup>-4</sup>	0.69 <sup>-5</sup>	0.36 <sup>-5</sup>	0.15 <sup>-5</sup>
140	0.173 <sup>-2</sup>	0.38 <sup>-3</sup>	0.42 <sup>-4</sup>	0.14 <sup>-4</sup>	0.57 <sup>-5</sup>	0.30 <sup>-5</sup>	0.12 <sup>-5</sup>
160	0.163 <sup>-2</sup>	0.37 <sup>-3</sup>	0.35 <sup>-4</sup>	0.13 <sup>-4</sup>	0.51 <sup>-5</sup>	0.27 <sup>-5</sup>	—
180	0.16 <sup>-2</sup>	—	—	—	—	—	—

† The superscripts to the numbers denote the power of 10 by which they should be multiplied.

expect the same situation to prevail for the  $1s \rightarrow 2s$  excitation in hydrogen. In figure 4 we compare the DWSBA cross section with the  $1s-2s-2p$  close-coupling calculation of Kingston *et al* (1976) at 54.4 eV. This figure reveals a striking difference between the DWSBA and close-coupling cross sections at all angles. Not only does the DWSBA lie well below the close-coupling cross section in the forward angular region, as anticipated, but also at most other angles. When integrated the differential cross sections of figure 4 lead to total cross sections differing by a factor of two. Of the two total cross sections the DWSBA value is the one in agreement with the available experimental data (see § 5.2.3 and table 7). It will be very interesting to see what light is thrown on this difference by future measurements of the  $1s \rightarrow 2s$  differential cross section.

There are no experimental measurements of the separate  $1s \rightarrow 2s$  and  $1s \rightarrow 2p$  differential cross sections at present. However, differential cross sections for exciting the  $n = 2$  level (i.e.  $1s \rightarrow 2s + 1s \rightarrow 2p$ ) have been determined. There are three sets of such cross sections in the energy range of interest to us (54.4 eV upwards): Williams (1969); Williams and Willis (1975) and White *et al* (1979). Williams (1969) measured only relative cross sections at 50, 100 and 200 eV. However, these results have been placed on an absolute scale by Bohm (1974). Williams and Willis (1975) measured absolute cross sections at 54.4, 100, 136, 200, 300 and 680 eV. These numbers agree



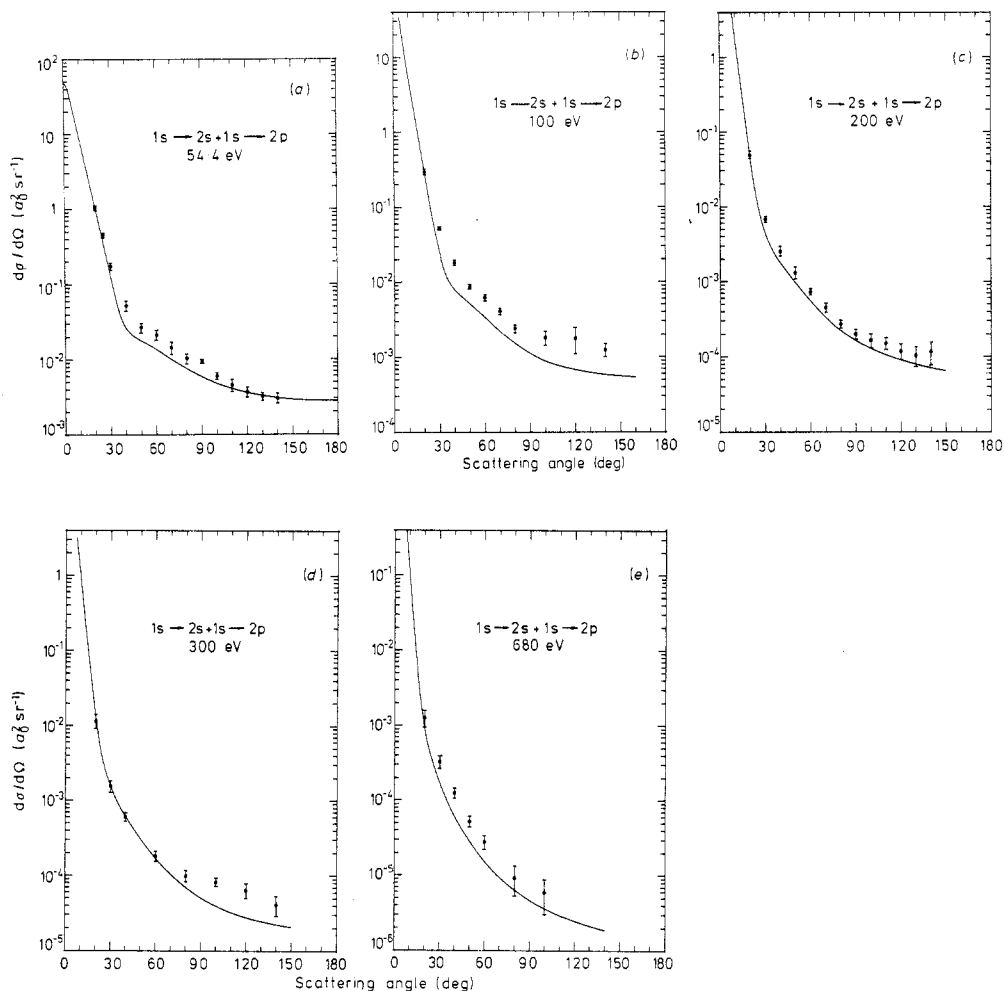
**Figure 4.** Differential cross sections for  $e^- + H(1s) \rightarrow e^- + H(2s)$  at 54.4 eV ( $k_0 = 2$  au). —, DWSBA; ---, close-coupling approximation of Kingston *et al* (1976).

with those of Williams (1969), as normalised by Bohm, within the combined experimental errors. While Williams and Williams and Willis have confined their data to angles greater than about  $20^\circ$  White *et al* have measured relative  $n = 2$  excitation cross sections at angles between  $7$  and  $20^\circ$ , and at energies of 136, 200 and 300 eV.

In figure 5, we compare the sum of our  $1s \rightarrow 2s$  and  $1s \rightarrow 2p$  DWSBA cross sections with the absolute data of Williams and Willis (1975). Except at 300 eV the agreement is not too good, the DWSBA cross section generally tending to lie below the experimental points. In view of this discrepancy let us examine what support there is for the Williams and Willis measurements.

As mentioned above, the data of Williams (1969), as normalised by Bohm, are in agreement with the Williams and Willis cross sections. However, White *et al* (1979) have criticised the Williams and Willis measurements. White *et al* found that their relative data agreed in shape with the FBA in the angular range  $7$  to  $20^\circ$  (and at their energies of 136, 200 and 300 eV). Assuming that the FBA was accurate for angles between  $0$  and  $7^\circ$  they concluded that the FBA was also correct over the larger angular range  $0$  to  $20^\circ$ . However, at 136, 200 and 300 eV the Williams and Willis  $20^\circ$  cross sections are only between 60% and 70% of the FBA values. Since the errors on the Williams and Willis  $20^\circ$  cross sections vary from 10% at 136 eV to 22% at 300 eV the Williams and Willis measurements are clearly in conflict with the conclusions of White *et al*, as these latter authors point out. While the DWSBA is in very good agreement with the FBA at  $0^\circ$ , the two cross sections differ significantly over the angular range  $0$  to  $20^\circ$ , contrary to the results of White *et al*. Furthermore, despite the general discord between the DWSBA and the cross sections of Williams and Willis, the DWSBA is nearly always in agreement with their  $20^\circ$  measurement. The DWSBA, White *et al* and Williams and Willis are all in profound disagreement with one another.

On the theoretical side, there are calculations in better agreement with the data of Williams and Willis than our DWSBA (see, for example, Byron and Latour 1976,



**Figure 5.** Differential cross sections for  $e^- + H(1s) \rightarrow e^- + H(2s + 2p)$ : —, DWSBA;  $\bullet$ , experimental data of Williams and Willis (1975).

Kingston *et al* 1976, Baluja *et al* 1978, Gien 1979). However the agreement obtained is erratic and we are left with the impression that it may be largely fortuitous. To illustrate this point of view let us consider the eikonal Born series (EBS) model of Byron and Latour (1976).

At 100 and 200 eV the EBS cross section is in better agreement with the experimental data than the DWSBA; however, at 300 eV the reverse is true. There are no published EBS cross sections at 54.4 and 680 eV; it would be interesting to see how the EBS approximation fared at these energies. Byron and Latour emphasise that in the large-angle region their EBS method is just a leading order approximation. Yet it is precisely in this angular domain where the EBS cross section scores its success with the experiment of Williams and Willis. Some evidence against the large-angle EBS cross section comes from the  $1^1S \rightarrow 2^1P$  and  $1^1S \rightarrow 2^1S$  transitions in He. Joachain and Winters (1977) have calculated the EBS cross section for the  $1^1S \rightarrow 2^1P$  transition and Byron and Joachain (1975) have used a version of the EBS model, admittedly not the same as, but



supposedly better than, that of Byron and Latour, to study the  $1^1\text{S} \rightarrow 2^1\text{S}$  excitation. For both transitions the EBS methods seem to overestimate the large angle experimental cross sections, at least at the lower energies (about 200 eV); furthermore, the angular range in which this overestimation takes place is, at 200 eV, beyond about  $40^\circ$ , i.e. more or less that angular region in which the EBS cross section for hydrogen is generally larger than that of the DWSBA and therefore in better agreement with the Williams and Willis data.

While being critical of such agreement as there is between theory and the experiment of Williams and Willis, we do not wish to assert that our DWSBA represents the ultimate standard of accuracy. What we do wish to convey, however, is an unease with the experimental results. Further independent measurements of the absolute  $n = 2$  excitation cross sections would be very useful.

**5.2.3. Total cross sections and polarisation of Lyman  $\alpha$  radiation.** In table 7 the DWSBA total cross section for the  $1s \rightarrow 2s$  transition is compared with the FBA, the close-coupling numbers of Kingston *et al* (1976) and with the experimental data of Kauppila *et al* (1970).

**Table 7.** Total cross sections for the process  $e^- + \text{H}(1s) \rightarrow e^- + \text{H}(2s)$  (in units of  $\pi a_0^2$ ).

Energy (eV)	Experimental values <sup>†</sup>	DWSBA	First Born	Close-coupling approximation of Kingston <i>et al</i> (1976)
54.4	$0.056 \pm 0.004$	0.0537	0.1019	0.101
100	$0.039 \pm 0.004$	0.0404	0.0578	0.0582
200	$0.029 \pm 0.003$	0.0250	0.0295	0.0300
300	$0.020 \pm 0.002$	0.0179	0.0198	0.0201
400	$0.015 \pm 0.002$	0.0139	0.0149	
500	$0.012 \pm 0.002$	0.0113	0.0120	
680	$0.009 \pm 0.002$	0.0085	0.0088	

<sup>†</sup> Measurements of Kauppila *et al* (1970) with  $1s \rightarrow 3p$  cascade contribution subtracted as described in text.

As mentioned previously (§ 5.2.1) we have calculated the  $1s \rightarrow 2s$  DWSBA cross section exactly<sup>‡</sup> only at energies up to and including 300 eV. At 100, 200 and 300 eV we found that the exact DWSBA total cross section was very well approximated by

$$\sigma^{\text{ECSSBA}} + 0.328(\sigma^{\text{DW}} - \sigma^{\text{ECSSBA}}) \quad (44)$$

where  $\sigma^{\text{ECSSBA}}$  and  $\sigma^{\text{DW}}$  are respectively the  $1s \rightarrow 2s$  total cross sections in the ECSSBA and in the Dewangan-Walters version of the DWSBA (§ 4). In table 7 the DWSBA numbers at 400 eV and above have been calculated according to (44).

The data of Kauppila *et al* do not represent the pure  $1s \rightarrow 2s$  excitation cross section; there is a significant cascade contribution to their measurements with the principal cascade coming from the  $3p$  state. It has been estimated (Kauppila *et al* 1970) that the experimental cross section corresponds to

$$\sigma(1s \rightarrow 2s) + 0.23\sigma(1s \rightarrow 3p) \quad (45)$$

<sup>‡</sup> See last paragraph of § 4.

where  $\sigma(1s \rightarrow 2s)$  and  $\sigma(1s \rightarrow 3p)$  are the pure 2s and 3p excitation cross sections. The experimental values given in table 7 are intended to represent the pure 2s excitation cross section. At 54.4 and 100 eV the 'experimental' numbers have been constructed by subtracting from the measurements of Kauppila *et al* the term  $0.23 \sigma(1s \rightarrow 3p)$  (see (45)) where  $\sigma(1s \rightarrow 3p)$  was taken to be the Glauber cross section of Tai *et al* (1970)<sup>†</sup>. In view of the good agreement between the Glauber approximation and experiment for the  $1s \rightarrow 2p$  excitation (Tai *et al*), at energies greater than 30 eV, we have some confidence in using this approximation for the 3p excitation. At 200 eV and above the FBA to (45) agrees well with the results of Kauppila *et al*. In table 7 the 'experimental' cross sections given at 200 eV and above are the first Born values for the  $1s \rightarrow 2s$  transition qualified by the experimental errors on the measured cross section (45) of Kauppila *et al* at these energies.

In connection with the data of Kauppila *et al* there are two further points worth making. Firstly, their cross section is not absolute. What is measured is, essentially, the ratio of the cross section (45) to the  $1s \rightarrow 2p$  excitation cross section; the  $1s \rightarrow 2p$  cross section of Long *et al* (1968) is then used to generate the values of (45). However, the 2p cross section of Long *et al* was placed on an absolute scale by normalisation to the FBA at 200 eV; we shall see below that the DWSBA indicates that this is an accurate normalisation procedure. Secondly, Cox and Smith (1971) have also reported measurements of the cross section (45) which, in the energy range of interest to us, support the data of Kauppila *et al*.

From table 7 we see that the DWSBA cross section for the  $1s \rightarrow 2s$  transition agrees very well with the experimental values, particularly at 54.4 and 100 eV where the experimental data differ noticeably from the FBA cross section (however, see below for some qualifying remarks). At higher energies the DWSBA numbers approach the FBA results from below. The close-coupling cross sections of Kingston *et al* (1976) are almost indistinguishable from the FBA at all the energies of table 7 and therefore disagree markedly with both experiment and the DWSBA at the lower energies. Even at an energy as high as 680 eV the DWSBA differs from the FBA by 3.5%.

In table 8 we compare the total cross section for the  $1s \rightarrow 2p$  transition,  $\sigma(1s \rightarrow 2p)$ , calculated in our DWSBA, the FBA and the close-coupling approximation (Kingston *et al* 1976) with the experimental data of Long *et al* (1968). Denoting by  $\sigma_m(1s \rightarrow 2p)$  the total cross section for exciting the 2p substate with magnetic quantum number  $m$ , where the direction of quantisation is taken to be along the direction of the incident electron beam (i.e.  $k_0$ ), we may write

$$\sigma(1s \rightarrow 2p) = \sigma_0(1s \rightarrow 2p) + 2\sigma_1(1s \rightarrow 2p). \quad (46)$$

(Note  $\sigma_{+1}(1s \rightarrow 2p) = \sigma_{-1}(1s \rightarrow 2p)$ .)

The DWSBA cross section has been exactly<sup>‡</sup> calculated only at 54.4, 100 and 200 eV (see § 5.2.1). At these energies it was discovered that the exact DWSBA cross section  $\sigma_0(1s \rightarrow 2p)$  was very well approximated by the Dewangan-Walters DWSBA cross section  $\sigma_0(1s \rightarrow 2p)$ , while the exact DWSBA cross section  $\sigma_1(1s \rightarrow 2p)$  was equally well given by the ECSSBA cross section  $\sigma_1(1s \rightarrow 2p)$ . The 'DWSBA' numbers at 300 eV and above, given in table 8, have been calculated from the Dewangan-Walters  $\sigma_0(1s \rightarrow 2p)$  and the ECSSBA  $\sigma_1(1s \rightarrow 2p)$  according to (46).

<sup>†</sup> Note that we have used the cross sections of figures 2 and 3 of Tai *et al* to perform this subtraction. We have not used the  $1s \rightarrow 3p$  cross section given in figure 6 of their paper; this latter cross section has been incorrectly plotted, e.g. the 3p threshold is incorrect.

<sup>‡</sup> See last paragraph of § 4.

**Table 8.** Total cross sections for the process  $e^- + H(1s) \rightarrow e^- + H(2p)$  (in units of  $\pi a_0^2$ ).

Energy (eV)	Experimental values <sup>†</sup>	DWSBA	First Born	Close-coupling approximation of Kingston <i>et al</i> (1976)
54.4	$0.79 \pm 0.01$	0.943	1.041	0.908
100	$0.67 \pm 0.02$	0.709	0.750	0.681
200	$0.48 \pm 0.01$	0.467	0.480	0.452
300		0.354	0.361	0.346
400		0.288	0.292	
500		0.244	0.247	
680		0.193	0.195	

<sup>†</sup> Total cross sections calculated from the measurement of Long *et al* (1968) using the Lyman  $\alpha$  polarisation fractions of Ott *et al* (1970). The values listed have been obtained by interpolation.

Another parameter of interest in connection with the  $1s \rightarrow 2p$  excitation is the polarisation fraction of the Lyman  $\alpha$  radiation  $P$  emitted when the excited  $2p$  state decays to the ground state. This parameter is defined by

$$P = \frac{I_{\parallel} - I_{\perp}}{I_{\parallel} + I_{\perp}} \quad (47)$$

where, when viewing the Lyman  $\alpha$  radiation emitted at  $90^\circ$  to the direction of the incident electron beam,  $I_{\parallel}$  and  $I_{\perp}$  are the radiation intensities with the electric vector parallel and perpendicular to the incident beam direction respectively. The right hand side of (47) may be rendered in terms of the cross sections  $\sigma_0(1s \rightarrow 2p)$  and  $\sigma_1(1s \rightarrow 2p)$  (Percival and Seaton 1958).

$$P = \frac{\sigma_0(1s \rightarrow 2p) - \sigma_1(1s \rightarrow 2p)}{2.375\sigma_0(1s \rightarrow 2p) + 3.749\sigma_1(1s \rightarrow 2p)} \quad (48)$$

The cross section measured by Long *et al* (1968) is not  $\sigma(1s \rightarrow 2p)$  but rather a quantity,  $Q_{\perp}$ , related to the total  $1s \rightarrow 2p$  cross section by

$$\sigma(1s \rightarrow 2p) = (1 - \frac{1}{3}P)Q_{\perp}. \quad (49)$$

To determine  $\sigma(1s \rightarrow 2p)$  from  $Q_{\perp}$  we therefore also need to know the polarisation fraction  $P$  as a function of impact energy. This is provided by the measurements of Ott *et al* (1970). Combining these results with the cross section of Long *et al* we have calculated from (49) the experimental  $1s \rightarrow 2p$  total cross section given in table 8.

Unlike the  $1s \rightarrow 2s$  data of Kauppila *et al* (1970), the  $1s \rightarrow 2p$  measurements are not clouded by a substantial cascade component; thus, it is estimated, in the neighbourhood of 200 eV cascade effects only account for about 2% of the measured cross section; however, below 100 eV cascade effects may be larger. The measured cross section  $Q_{\perp}$  is not absolute; it has been placed on an absolute scale by Long *et al* through normalisation to the FBA at 200 eV (with a 2% allowance for cascade).

From table 8 we see that the DWSBA cross sections at 100 and 200 eV are close to the experimental values, although not in agreement within experimental error. However, at 54.4 eV the DWSBA result is noticeably larger. This casts some doubt upon the perfect agreement between the DWSBA cross section and experiment for the  $1s \rightarrow 2s$

transition at 54.4 eV, shown in table 7: if, at 54.4 eV, the experimental  $1s \rightarrow 2p$  cross section is in error then so is the corresponding  $1s \rightarrow 2s$  result since their normalisations are linked; on the other hand, if the DWSBA  $1s \rightarrow 2p$  cross section is in error, it would be surprising if the DWSBA  $1s \rightarrow 2s$  result were not also inaccurate.

The DWSBA supports the normalisation of the experimental data to the FBA at 200 eV; at this energy the DWSBA lies only 3% below the FBA value. We note here, once more, that the experimental  $1s \rightarrow 2s$  total cross section of table 7 rests upon the validity of this normalisation procedure. Indeed the validity of normalising the  $1s \rightarrow 2p$  cross section to the FBA at 200 eV has been a matter of some discussion (see, for example, Geltman and Burke 1970, Damburg and Propin 1972). Thus Damburg and Propin, on the basis of a model calculation, warn that the FBA could be in error by as much as 20% in the range 200 to 1000 eV. Clearly, neither our DWSBA results nor the close-coupling cross section of Kingston *et al* (1976) (see table 8) support this conclusion, although the close-coupling numbers do indicate a greater deviation from the FBA. In our opinion, the fallacy in the Damburg–Propin model lies in the use of potentials which are singular as  $r_0^{-2}$  as  $r_0$  tends to zero, even though these authors do make some allowance for this singularity by ignoring the lowest three partial waves.

The close-coupling numbers of Kingston *et al* (1976) appear to be in marginally better agreement with experiment at 100 and 54.4 eV than the DWSBA. However, remembering that experiment is normalised to the FBA at 200 eV, we see that a more proper comparison would be to normalise the experiment to the close-coupling results at 200 eV. When this is done the close-coupling approximation is found to deviate from experiment by as much as the DWSBA; indeed between 54.4 and 300 eV the DWSBA and close-coupling cross sections differ essentially only in normalisation, i.e. they have the same shape; the shape of the experimental cross section in this energy range is noticeably different from both theories and in the opposite direction to that which we would expect if distortion by cascade effects were the explanation of the difference between theory and experiment.

In table 9 we compare the polarisation fraction of the Lyman  $\alpha$  radiation  $P$  measured by Ott *et al* (1970) with the corresponding FBA and DWSBA results. As mentioned earlier the DWSBA numbers at 54.4, 100 and 200 eV are exact†. At 300 eV and above the 'DWSBA' polarisation fraction has been calculated from (48) using the Dewangan–Walters DWSBA cross section for  $\sigma_0(1s \rightarrow 2p)$  and the ECSSBA values for

Table 9. Polarisation fraction of Lyman  $\alpha$  radiation.

Energy (eV)	Experiment (Ott <i>et al</i> 1970)	DWSBA	First Born
54.4	+0.12 ± 0.01‡	+0.135	+0.088
100	+0.05 ± 0.01	+0.050	+0.027
200	0.00 ± 0.01	−0.013	−0.023
300	−0.03 ± 0.02	−0.040	−0.046
400	−0.03 ± 0.02	−0.058	−0.060
500	−0.05 ± 0.02	−0.070	−0.070
680	−0.06 ± 0.02‡	−0.084	−0.082

‡ Interpolated values.

† See last paragraph of § 4.

$\sigma_1(1s \rightarrow 2p)$ , this should be a very good approximation to the exact DWSBA results, see above. From table 9 we see that the DWSBA numbers are an improvement on the FBA values; agreement with experiment is not quite perfect.

## 6. Conclusions

We have shown that the approximations of Dewangan and Walters (1977) and of Winters (1978) for simplifying the calculation of distorted-wave second Born amplitudes are accurate for elastic electron-hydrogen scattering at high enough energies (and also for  $e^-$ -He scattering, see § 5.1.1 and Bransden *et al* 1978). However, both approximations are unreliable for inelastic scattering. The failure of the Winters method for inelastic scattering is a warning to all those working with local second-order potentials.

For elastic electron-hydrogen scattering we have obtained fairly good agreement between the DWSBA and experiment. The agreement is consistent with previous work on He and Ne (Dewangan and Walters 1977). However, for the  $n = 2$  excitation there is a disturbing discord between our DWSBA and the experimental data of Williams and Willis (1975). The irony is that there are simpler approximations in better agreement with the data (see, for example, Kingston *et al* 1976, Baluja *et al* 1978). Unless there is some conspiracy of cancellation amongst the effects neglected by these simpler approximations it is difficult to see how this agreement can be anything but fortuitous. What is needed are further independent experiments on the  $n = 2$  transitions and further experience with the DWSBA on inelastic transitions in atomic systems other than hydrogen.

## References

- Baluja K L, McDowell M R C, Morgan L A and Myerscough V P 1978 *J. Phys. B: Atom. Molec. Phys.* **11** 715-26
- Bethe H A and Salpeter E E 1957 *Quantum Mechanics of One- and Two- Electron Atoms* (Berlin: Springer)
- Bohm B 1974 *PhD Thesis* University of Adelaide, South Australia
- Bonham R A 1971a *Phys. Rev. A* **3** 298-309
- 1971b *Phys. Rev. A* **3** 1958-68
- Bransden B H and Coleman J P 1972 *J. Phys. B: Atom. Molec. Phys.* **5** 537-45
- Bransden B H and Dewangan D P 1979 *J. Phys. B: Atom. Molec. Phys.* **12** 1377-89
- Bransden B H, Smith J J and Winters K H 1978 *J. Phys. B: Atom. Molec. Phys.* **11** 3095-114
- Buckley B D and Walters H R J 1974 *J. Phys. B: Atom. Molec. Phys.* **7** 1380-400
- 1975 *J. Phys. B: Atom. Molec. Phys.* **8** 1693-715
- Byron F W Jr and Joachain C J 1973 *Phys. Rev. A* **8** 1267-82
- 1974 *Phys. Rev. A* **9** 2559-68
- 1975 *J. Phys. B: Atom. Molec. Phys.* **8** L284-8
- 1977a *J. Phys. B: Atom. Molec. Phys.* **10** 207-26
- 1977b *Phys. Rev. A* **15** 128-46
- Byron F W Jr and Latour L J Jr 1976 *Phys. Rev. A* **13** 649-64
- Cox D M and Smith S J 1971 *Proc. 7th Int. Conf. on Physics of Electronic and Atomic Collisions* (Amsterdam: North-Holland) Abstracts pp 707-8
- Damburg R J and Geltman S 1968 *Phys. Rev. Lett.* **20** 485-7
- Damburg R and Propin R 1972 *J. Phys. B: Atom. Molec. Phys.* **5** 533-6
- Dewangan D P and Walters H R J 1977 *J. Phys. B: Atom. Molec. Phys.* **10** 637-61
- Ermolaev A M and Walters H R J 1979 *J. Phys. B: Atom. Molec. Phys.* **12** L779-84
- Furness J B and McCarthy I E 1973 *J. Phys. B: Atom. Molec. Phys.* **6** 2280-91

- Geltman S and Burke P G 1970 *J. Phys. B: Atom. Molec. Phys.* **3** 1062–72
- Gien T T 1979 *Phys. Rev. A* **20** 1457–67
- de Heer F J, McDowell M R C and Wagenaar R W 1977 *J. Phys. B: Atom. Molec. Phys.* **10** 1945–53
- Holt A R 1972 *J. Phys. B: Atom. Molec. Phys.* **5** L6–8
- Holt A R and Moiseiwitsch B L 1968 *J. Phys. B: Atom. Molec. Phys.* **1** 36–47
- Joachain C J and Vanderpoorten R 1973 *J. Phys. B: Atom. Molec. Phys.* **6** 622–41
- Joachain C J and Winters K H 1977 *J. Phys. B: Atom. Molec. Phys.* **10** L727–30
- Kauppila W E, Ott W R and Fite W L 1970 *Phys. Rev. A* **1** 1099–108
- Kingston A E, Fon W C and Burke P G 1976 *J. Phys. B: Atom. Molec. Phys.* **9** 605–18
- Lloyd C R, Teubner P J O, Weigold E and Lewis B R 1974 *Phys. Rev. A* **10** 175–81
- Long R L, Cox D M and Smith S J 1968 *J. Res. NBS A* **72** 521–35
- McDowell M R C 1980 *Comm. Atom. Molec. Phys.* **9** 127–41
- Madison D H 1980 *Coherence and Correlation in Atomic Collisions*, ed H Kleinpoppen and J F Williams (New York: Plenum) p 167
- Moiseiwitsch B L 1963 *Proc. Nat. Acad. Sci. India* **33** 537–42
- Ott W R, Kauppila W E and Fite W L 1970 *Phys. Rev. A* **1** 1089–98
- Percival I C and Seaton M J 1958 *Phil. Trans. R. Soc. A* **251** 113–38
- Prasad K 1964 *PhD Thesis* The Queen's University of Belfast
- Rose M E 1957 *Elementary Theory of Angular Momentum* (New York: Wiley)
- Tai H, Bassel R H and Gerjuoy E 1970 *Phys. Rev. A* **1** 1819–35
- Vanderpoorten R 1975 *J. Phys. B: Atom. Molec. Phys.* **8** 926–39
- Vanderpoorten R and Winters K H 1978 *J. Phys. B: Atom. Molec. Phys.* **11** 281–92
- 1979 *J. Phys. B: Atom. Molec. Phys.* **12** 473–88
- Walters H R J 1976a *Comm. Atom. Molec. Phys.* **5** 173–83
- 1976b *J. Phys. B: Atom. Molec. Phys.* **9** 227–37
- White M D, Ross K J and Bolouri H 1979 *J. Phys. B: Atom. Molec. Phys.* **12** 811–7
- Williams J F 1975 *J. Phys. B: Atom. Molec. Phys.* **8** 2191–9
- Williams J F and Willis B A 1975 *J. Phys. B: Atom. Molec. Phys.* **8** 1641–69
- Williams K L 1969 *Proc. 6th Int. Conf. on Physics of Electronic and Atomic Collisions* (Cambridge, Mass.: MIT) Abstracts pp 731–4
- van Wingerden B, Weigold E, de Heer F J and Nygaard K J 1977 *J. Phys. B: Atom. Molec. Phys.* **10** 1345–62
- Winters K H 1978 *J. Phys. B: Atom. Molec. Phys.* **11** 149–65
- 1979 *Comm. Atom. Molec. Phys.* **8** 93–101
- Winters K H, Clark C D, Bransden B H and Coleman J P 1974 *J. Phys. B: Atom. Molec. Phys.* **7** 788–98
- Wollings M J 1972 *J. Phys. B: Atom. Molec. Phys.* **5** L164–6