

A second-order potential for the elastic scattering of electrons by atomic hydrogen

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Abstract. A second-order equivalent (optical) potential for elastic scattering has been constructed by expanding the intermediate states in a set of pseudostates, avoiding the closure approximation used in the method of Bransden and Coleman. Using this potential the differential cross section for the elastic scattering of electrons by atomic hydrogen has been calculated for a number of energies in the range 1 to 100 eV. Good agreement is obtained with experimental data of Williams except at small angles in the interval 8–30 eV for which the calculated cross section is larger than the data. A comparison is made with the results of other models and possible improvements are discussed.

1. Introduction

In this paper we develop a method of computing elastic scattering cross sections for electron–hydrogen–atom collisions at electron impact energies ranging from very low energies (~ 1 eV) to the high-energy region (>100 eV) (excluding Feshbach resonances). During recent years a number of theoretical models have been developed to handle elastic scattering in this intermediate-energy region, among them the algebraic variational method of Callaway and Wooten (1974), the eikonal Born series of Byron and Joachain (1973a,b, 1974b, 1977b) and various optical potential approaches (Vanderpoorten 1975, Winters *et al* 1974, Byron and Joachain 1974a, 1977a, Alton *et al* 1972). Further details and a review of these methods have been presented in the articles by Bransden and McDowell (1977, 1978), and by Byron and Joachain (1977c).

It is our aim in the present paper to extend the second-order optical potential method of Bransden and Coleman (1972) in such a way that it may be applied to lower incident energies than those considered by Winters *et al* (1974) and to compare the resulting differential and total cross sections with absolute experimental data where available. In particular we shall compare our results for differential cross sections with the absolute measurements of Williams (1975a,b).

2. General formulation

Although the second-order optical potential theory of Bransden and Coleman (1972) has been described elsewhere in a series of papers by Bransden and co-workers, we present here a brief summary of the theory for completeness.

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We assume that the atomic nucleus, carrying a general charge Z , is at rest throughout the collision and we measure position vectors relative to this point. Atomic units will be used throughout except where specified.

Writing \mathbf{r} for the atomic electron coordinates and \mathbf{x} for the incident electron, we can write the Schrödinger equation for the total colliding system as

$$(H - E)\Psi(\mathbf{r}, \mathbf{x}) = 0 \quad (2.1)$$

where $\Psi(\mathbf{r}, \mathbf{x})$ denotes the total wavefunction and the Hamiltonian H is given by

$$H = -\frac{1}{2}\nabla_r^2 - \frac{1}{2}\nabla_x^2 - \frac{Z}{r} - \frac{Z}{x} + \frac{1}{|\mathbf{r} - \mathbf{x}|}.$$

Expanding $\Psi(\mathbf{r}, \mathbf{x})$ in terms of the atomic eigenstates $\phi_n(\mathbf{r})$, we have that

$$\Psi(\mathbf{r}, \mathbf{x}) = \sum_n \phi_n(\mathbf{r}) F_n(\mathbf{x}) \quad (2.2)$$

where for clarity exchange has been omitted. Terms arising from exchange will, however, be included in the final equations.

By substituting (2.2) into the Schrödinger equation (2.1) and projecting out onto the states $\phi_n(\mathbf{r})$ we derive the usual set of coupled equations

$$(\nabla^2 + k_n^2)F_n(\mathbf{x}) = \sum_{m=0}^M V_{nm}(\mathbf{x})F_m(\mathbf{x}) + \sum_{m=M+1}^{\infty} V_{nm}(\mathbf{x})F_m(\mathbf{x}) \quad n = 0, 1, \dots \quad (2.3)$$

to be solved for the channel functions $F_n(\mathbf{x})$. The channel energy is given by

$$k_n^2 = 2(E - \varepsilon_n)$$

with ε_n the energy corresponding to eigenstate ϕ_n , and for 'open' channels $k_n^2 > 0$, while for 'closed' channels $k_n^2 < 0$. The potential matrix V_{nm} is defined by

$$V_{nm}(\mathbf{x}) = \langle \phi_n(\mathbf{r}) | V(\mathbf{r}, \mathbf{x}) | \phi_m(\mathbf{r}) \rangle$$

where

$$V(\mathbf{r}, \mathbf{x}) = -\frac{2Z}{x} + \frac{2}{|\mathbf{r} - \mathbf{x}|}.$$

It is to be noted that the summation over m in equations (2.3) covers the discrete and continuum states of the target atom. Our aim is to solve equations (2.3) for a restricted number of F_n , $n = 0, \dots, M$, while at the same time taking into account the effect of other channels, $m > M$, and for this purpose it is convenient to separate the right-hand side of equation (2.3) into two distinct sums as indicated.

For the case $m > M$, we approximate equations (2.3) by

$$(\nabla^2 + k_m^2)F_m(\mathbf{x}) = \sum_{q=0}^M V_{mq}(\mathbf{x})F_q(\mathbf{x}).$$

This equation may be solved formally for $F_m(\mathbf{x})$:

$$F_m(\mathbf{x}) = \sum_{q=0}^M \int G_0(\mathbf{x}, \mathbf{r}; k_m^2) V_{mq}(\mathbf{r}) F_q(\mathbf{r}) d\mathbf{r} \quad m > M$$

where the free-particle Green's function is defined as

$$G_0(\mathbf{x}, \mathbf{r}; k_m^2) = \frac{-\exp(+ik_m|\mathbf{x} - \mathbf{r}|)}{4\pi|\mathbf{x} - \mathbf{r}|}$$

and satisfies outgoing wave boundary conditions, in the 'open' channels $k_m^2 > 0$.

Returning to equation (2.3), we find on substituting for $F_m(\mathbf{x})$, $m > M$:

$$(\nabla^2 + k_n^2)F_n(\mathbf{x}) = \sum_{m=0}^M V_{nm}(\mathbf{x})F_m(\mathbf{x}) + \sum_{q=0} \int K_{nq}(\mathbf{x}, \mathbf{r})F_q(\mathbf{r}) d\mathbf{r} \quad (2.4)$$

where

$$K_{nq}(\mathbf{x}, \mathbf{r}) = \sum_{m=M+1}^{\infty} V_{nm}(\mathbf{x})G_0(\mathbf{x}, \mathbf{r}; k_m^2)V_{mq}(\mathbf{r}). \quad (2.5)$$

The quantity K_{nq} is an equivalent potential matrix calculated to second order in the interaction $V(\mathbf{r}, \mathbf{x})$. Third and higher order contributions to K_{nq} are easily written down (see Bransden and McDowell 1977), but are difficult to compute in general. However, the diagonal interactions V_{mm} ($m > M$), which give rise to an important subset of third and higher order terms can be taken into account by replacing the free-particle Green's functions G_0 by a Hartree (or Hartree-Fock) Green's function G_{HF} , as in the work of Scott and Taylor (1979a,b).

3. Single-channel model

Specialising to the single-channel case, obtained by putting $M = 0$ in equations (2.4) and (2.5), we find that

$$\begin{aligned} (\nabla^2 + k_0^2)F_0^\pm(\mathbf{x}) &= V_{00}(\mathbf{x})F_0^\pm(\mathbf{x}) + \int W_{00}^\pm(\mathbf{x}, \mathbf{r})F_0^\pm(\mathbf{r}) d\mathbf{r} + \int K_{00}(\mathbf{x}, \mathbf{r})F_0^\pm(\mathbf{r}) d\mathbf{r} \\ &\quad + \int L_{00}^\pm(\mathbf{x}, \mathbf{r})F_0^\pm(\mathbf{r}) d\mathbf{r} \end{aligned} \quad (3.1)$$

where $V_{00}(\mathbf{x})$ is the usual static potential appearing in equation (2.3) and $W_{00}^\pm(\mathbf{x}, \mathbf{r})$ is the corresponding exchange potential given by

$$W_{00}^\pm(\mathbf{x}, \mathbf{r}) = \pm \phi_0^*(\mathbf{r})\phi_0(\mathbf{x}) \left((2\varepsilon_0 - k_0^2) + \frac{2}{|\mathbf{r} - \mathbf{x}|} \right). \quad (3.2)$$

The upper sign is chosen for the singlet and the lower sign for the triplet spin configuration. The second-order direct potential K_{00} reduces to the form

$$K_{00}(\mathbf{x}, \mathbf{r}) = \sum_{m=1}^{\infty} \langle \phi_0 | V | \phi_m \rangle G_0(k_m^2) \langle \phi_m | V | \phi_0 \rangle. \quad (3.3)$$

Some feeling for the importance of both the second-order exchange potential L_{00}^\pm and of the diagonal interactions V_{mm} can be obtained from the work of Scott and Taylor (1979a,b) on the elastic scattering of electrons by helium. In that work an optical potential was constructed either using the free-particle Green's function G_0 or a Hartree-Fock Green's function G_{HF} . It was found that the difference was insignificant

at the higher energies $E > 30$ eV and relatively small at lower energies. While recognising that second-order exchange and diagonal interaction terms might well be more important in hydrogen than in helium, it was decided to neglect L_{00}^{\pm} and employ the free-particle Green's function in the present work, which enables a direct comparison between our results and those of Winters *et al* (1974) at the higher energies and of Coulter and Garrett (1978) at the lowest energies.

3.1. Closure

In the original applications of the model of Bransden and Coleman the second-order potential was evaluated approximately using closure. In this approach the first N low-lying terms in the sum (3.3) are determined exactly and for $m > N$, the intermediate energy $\frac{1}{2}k_m^2$, appearing as the argument of the Green's function, is replaced by a fixed, average, energy $\frac{1}{2}\bar{k}^2$. It is then found that K_{00} is given by

$$K_{00}(\mathbf{x}, \mathbf{r}) = \sum_{m=1}^N \langle \phi_0 | V(\mathbf{y}, \mathbf{x}) | \phi_m \rangle G_0(k_m^2) \langle \phi_m | V(\mathbf{y}, \mathbf{r}) | \phi_0 \rangle \\ + G_0(\bar{k}^2) \left(\langle \phi_0 | V(\mathbf{y}, \mathbf{x}) V(\mathbf{r}, \mathbf{y}) | \phi_0 \rangle \right. \\ \left. - \sum_{m=0}^N \langle \phi_0 | V(\mathbf{y}, \mathbf{x}) | \phi_m \rangle \langle \phi_m | V(\mathbf{y}, \mathbf{r}) | \phi_0 \rangle \right).$$

The average energy \bar{k}^2 can be chosen in various ways to satisfy some physical condition. It is often chosen so that at large distances the real part of the interaction is given correctly in terms of the known dipole polarisability of the target atom. This was the choice made by Winters *et al* (1974) in their work using the Bransden and Coleman model. Although calculations by Ermolaev and Walters (1979) using the second Born approximation have shown that, at least for elastic scattering, the closure approximation can be expected to be accurate down to at least 30 eV, it is essentially a high-energy approximation and one of the objectives of the present work is to see whether it can be avoided by using intermediate pseudostates.

3.2. Pseudostates

In an alternative treatment, the part of the wavefunction corresponding to channels $m \geq M+1$, which contains an integration over the continuum states is expanded in terms of a discrete set of functions $\Phi_n(\mathbf{r})$ containing no continuum. If a finite number of terms are used as an approximation

$$\int dn \phi_n(\mathbf{r}) F_n(\mathbf{x}) \approx \sum_{n=m+1}^N \Phi_n(\mathbf{r}) F_n(\mathbf{x})$$

we have, in effect, generated a quadrature formula for the integration over the continuum states. There is no unique choice for the pseudostate functions Φ_n . A convenient choice, which we have adopted here, is that of Callaway and Wooten (1974), who have taken Φ_m to be linear combinations of Slater orbitals, so that the functions Φ_m diagonalise the Hamiltonian H_T of the target atom:

$$\langle \Phi_n | -\frac{1}{2}\nabla_r^2 - r^{-1} | \Phi_m \rangle = \bar{\epsilon}_m \delta_{nm}.$$

Using a set of N such functions, the second-order potential becomes

$$K_{00}(\mathbf{x}, \mathbf{r}) = \sum_{m=1}^N \langle \phi_0 | V | \Phi_m \rangle G_0(\bar{k}_m^2) \langle \Phi_m | V | \phi_0 \rangle \quad (3.4)$$

where

$$\bar{k}_m^2 = 2(\varepsilon - \bar{\varepsilon}_m).$$

We investigated several sets of such functions to determine the minimum set consistent with an adequate representation of the intermediate states, being guided by the results of similar work for proton excitation of hydrogen by Bransden *et al* (1979). Each pseudostate set contained the exact 2s, 2p and 3d hydrogenic functions together with functions for which the energies $\bar{\varepsilon}_n$ were positive and which overlapped the hydrogenic continuum. The p functions were required to reproduce the correct long-range dipole behaviour of the real part of the optical potential. Each pseudostate has the radial form

$$\phi_m^{(i)}(r) = \sum_{a=1}^A c_a^{(i)} r^{n_a} \exp(-\alpha_a r)$$

where the coefficients $c_a^{(i)}$ are obtained from the diagonalisation of H_T . Our final set of pseudostates adopted for the calculations reported in this paper comprised 5 s orbitals, 4 p orbitals, 4 d orbitals and 3 f orbitals, details of which are given in table 1. We note that the 1s state is excluded from the summation (3.4) but that this does not prohibit us from incorporating such a Slater-type orbital into a primitive basis used to construct the pseudostates, provided the orthogonality conditions $\langle \phi_{1s} | \phi_m \rangle = 0$ for $m = 1, 2, \dots, N$ are all satisfied.

3.3. Numerical methods

In order to proceed further with the solution of equation (3.1), we insert the usual

Table 1. The parameters of the pseudostates. The notation is defined in the text.

Orbital type	a	n_a	α_a	E_m^i (Ryd)
s symmetry	1	0	0.2	-0.25
	2	0	0.5	-0.11
	3	1	0.5	-0.02
	4	0	0.8	0.42
	5	1	0.8	3.68
	6	0	1.0	
p symmetry	1	1	0.5	-0.25
	2	1	0.8	-0.08
	3	2	0.8	0.30
	4	1	1.0	2.19
d symmetry	1	2	0.33	-0.11
	2	2	0.5	-0.03
	3	2	1.2	0.41
	4	2	1.2	2.44
f symmetry	1	3	0.25	-0.06
	2	3	1.0	0.33
	3	3	1.5	2.26

partial-wave expansions for $F_0(\mathbf{x})$ and $G_0(\mathbf{x}, \mathbf{r}; k^2)$:

$$F_0(\mathbf{x}) = \sum_l a_l \frac{F_l(x)}{x} Y_{l0}(\hat{x})$$

$$G_0(\mathbf{x}, \mathbf{r}; k^2) = \sum_{l,m} \frac{G_l(x, r; k^2)}{xr} Y_{lm}^*(\hat{x}) Y_{lm}(\hat{r}).$$

The appropriate expression for the free-particle partial-wave Green's function is selected according to the sign of the channel energy k^2 . For open channels, we take

$$G_l(x, r; k^2) = -k^{-1} \hat{j}_l(kr_{<}) (\hat{n}_l(kr_{>}) + i \hat{j}_l(kr_{>}))$$

while in the case of closed channels

$$G_l(x, r; k^2) = -\frac{2k}{\pi} x r i_l(kr_{<}) k_l(kr_{>}).$$

In these expressions, \hat{j}_l and \hat{n}_l are regular and irregular spherical Bessel functions and i_l and k_l modified spherical Bessel functions of the first and third kind. We denote by $r_{<}$ and $r_{>}$ the lesser and greater respectively of r and x .

Carrying out the partial-wave analysis and adopting the notation of Percival and Seaton (1957), we find

$$\left(\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} + k^2 \right) F_l(r)$$

$$= \left(-\frac{2Z}{r} + 2y_0(x\phi_{1s}, x\phi_{1s}|r) \right) F_l(r)$$

$$\pm \left(\delta_{l0}(2\varepsilon_{1s} - k^2) \Delta(x\phi_{1s}, F_l) + \frac{2}{2l+1} y_l(x\phi_{1s}, F_l|r) \right) r\phi_{1s}(r)$$

$$+ 4 \sum_{L=s}^f \sum_{\lambda l_1 l_2} f_\lambda(l_1 l_2, 0l; l)^2 B_l(\lambda l_1 l_2, L; r) \quad (3.5)$$

where

$$B_l(\lambda l_1 l_2, L; r) = \sum_{n=1}^{N_L} y_\lambda(x\phi_{1s}, x\Phi_{nL}|r) \int_0^\infty G_{l_2}(r, x_1; k_n^2) y_\lambda(x_2\Phi_{nL}, x_2\phi_{1s}|x_1) F_l(x_1) dx_1. \quad (3.6)$$

The potential terms on the right-hand side of equation (3.5) correspond, respectively, to the first-order static potential and its exchange counterpart with appropriate sign and the second-order terms comprising the direct component of the optical potential—second-order exchange terms will be included in a later study. With our choice of pseudostate basis, we have in equation (3.6) that $N_s = 5$, $N_p = 4$, $N_d = 4$ and $N_f = 3$. Equation (3.5) is an integro-differential equation involving a complex and energy-dependent non-local potential.

Our overall approach to solving this equation has been to proceed by iteration. The initial solution is computed omitting the non-local terms and using the de Vogelaere algorithm (de Vogelaere 1955), as coded by Chandra (1973) and subsequently modified by McCarthy and McDowell (1979) to handle complex potentials, to integrate the equation. At the same time we build up the non-local terms ready to use as input for the next iteration. The non-local term then forms an inhomogeneous term in the equation

which is solved again to give a new iterate. This is repeated until the sum of the differences at each grid point between successive iterations is less than ε where typically $\varepsilon = 0.001$, that is

$$\left(\sum_{\nu} |F_{\nu}^{\text{old}} - F_{\nu}^{\text{new}}| \right) \left(\sum_{\nu} |F_{\nu}^{\text{new}}| \right)^{-1} < \varepsilon.$$

For an impact energy of 100 eV we find that 4 iterations are sufficient for $0 \leq l \leq 7$. Exchange is omitted when the singlet and triplet phaseshifts differ by less than 0.0001. At lower impact energies difficulty was encountered in obtaining a convergent solution for the singlet and triplet s waves due to the presence of the non-local exchange terms. The lower the energy the more iterations were required to achieve convergence. This problem was, however, overcome by modifying the code to allow for exchange exactly in the case of the s wave by introducing a further differential equation for $y_0(x\phi_{1s}, F_0|r)$ as discussed by Burke and Seaton (1971).

Having obtained a convergent solution out to some asymptotic point, typically $22 a_0$, we then impose the asymptotic boundary conditions to determine scattering parameters using the ASYM package due originally to Norcross (1969).

In order to compute differential and total cross sections, equation (3.5) was solved for up to 31 partial waves ($0 \leq l \leq 30$) with higher l values being taken into account through the polarised Born approximation. This involved subtracting from the scattering amplitude the partial-wave contributions computed in the polarised Born approximation and adding the complete polarised Born amplitude which was calculated in closed form. Further details of this technique in connection with e -H collisions are given by McDowell *et al* (1975).

4. Numerical results

The second-order potential model using intermediate pseudostates can be formulated as an approximation to the equations of the close-coupling model using the same pseudostates. Thus our results for elastic scattering are an approximation to those of a 17-state close-coupling model. The results of such a model are not available for comparison; but we can obtain some idea of the accuracy to be expected by comparing the results of a three-state ($1s$ - $2s$ - $2p$) close-coupling model, with those obtained from a second-order potential in which the only intermediate states retained are the $2s$ and $2p$ hydrogenic states. Such a comparison is shown in table 2 at an incident energy of 100 eV, both with and without exchange terms, for the lower-order partial-wave T -matrix elements, where $T_l = \exp(2i\sigma_l) - 1$ and σ_l is a complex phaseshift. The agreement is remarkably close, which supports the view that high-order components of the optical potential are small at this energy, and similar results are found at lower energies.

Our main results are shown in figures 1 and 2, where the computed differential cross sections[†] for incident energies of 1.22, 3.4, 8.7, 20, 30, 50 and 100 eV are shown compared with the experimental data of Williams (1975a, b). At the lowest energy, the calculated cross section is entirely consistent with the data, but at 3 eV and up to 30 eV the calculated cross section lies above the data at angles $\theta \leq 30^\circ$. At 50 eV the agreement with the data is very close, while at 100 eV close agreement in shape is

[†] Numerical tabulations of the computed cross sections can be obtained from the authors.

Table 2. T matrix (1s-1s element) at 100 eV.

<i>L</i>	1s-2s-2p close coupling	Optical potential (2s and 2p intermediate states only)
(a) No exchange		
0	-0.645, 0.910	-0.661, 0.909
1	-0.136, 0.467	-0.143, 0.465
2	-0.041, 0.222	-0.047, 0.223
3	-0.021, 0.107	-0.026, 0.109
4	-0.017, 0.053	-0.020, 0.056
5	-0.015, 0.028	-0.017, 0.030
(b) With exchange, singlet		
0	-0.520, 0.840	-0.537, 0.852
1	-0.093, 0.357	-0.094, 0.362
2	-0.033, 0.155	-0.035, 0.159
3	-0.022, 0.071	-0.022, 0.075
(c) With exchange, triplet		
0	-0.769, 0.956	-0.782, 0.945
1	-0.190, 0.565	-0.201, 0.557
2	-0.055, 0.287	-0.964, 0.284
3	-0.023, 0.143	-0.030, 0.143

obtained, but the experimental curve lies a little above the calculated values. The general characteristics of the data are well reproduced over the whole energy range, but it should, of course, be noted that the resonances lying below inelastic thresholds cannot be reproduced without the addition of certain third-order terms in the optical potential.

At 100 eV our results are very close to those of Winters *et al* (1974) with some small difference at large angles (see figure 2(c)) indicating that closure is a satisfactory approximation at this energy. At higher energies our results should be identical with those published by Winters *et al*. Also shown for comparison at 100 eV are the eikonal-Born series results of Byron and Joachain (1974a, b), which also depend on the closure approximation and which are in close agreement with the present results except at large angles. At the three energies of 20, 30 and 100 eV our results are compared with a two-state close-coupling model of Fon *et al* (1978), in which one pseudostate designated 2p was employed. Their results agree rather well with the data at 20 and 30 eV at angles less than about 60°, but are less satisfactory than the present results at larger angles.

The three lowest energies of 1.22, 3.4 and 8.7 eV are all below the $n = 2$ threshold, so that the potential is purely real. At these three energies Coulter and Garrett (1978) have also computed differential cross sections from the second-order potential model. However in their work the exact discrete and continuum hydrogenic intermediate states were employed in constructing the potential, which should be exact (to second order). As far as can be judged from a comparison of graphs, the results of Coulter and Garrett agree completely with our own, and the computed total cross sections are virtually identical (see table 3), which establishes that our pseudostate set represents the intermediate states to sufficient accuracy in the low-energy region. The importance of the long-range second-order polarisation potential is well known, but we have included the results of a first-order (static-exchange) potential calculation in figure 1(a)-(c), which omits this interaction, for comparison.

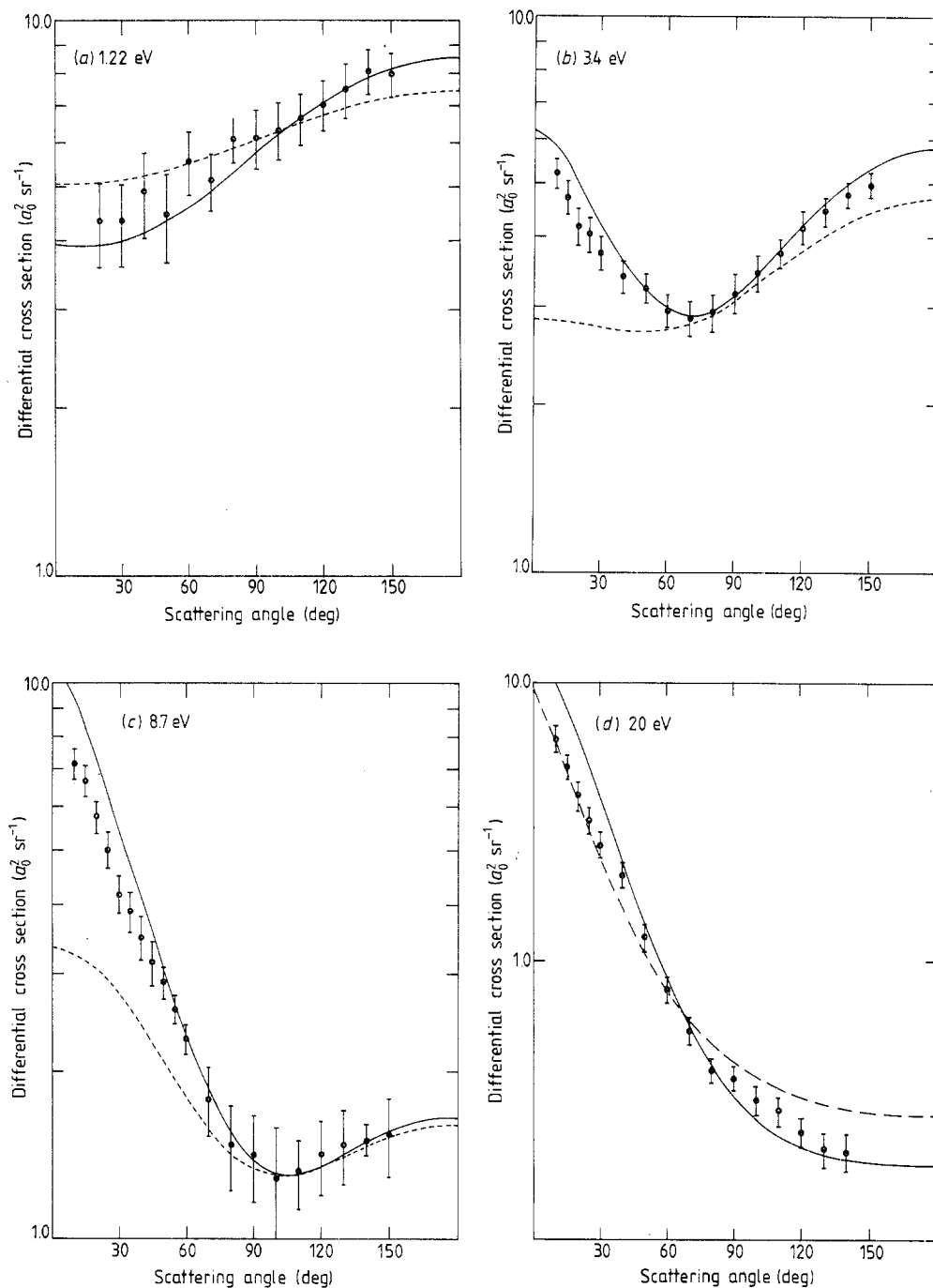


Figure 1. Differential cross sections for the elastic scattering of electrons by atomic hydrogen at (a) 1.22, (b) 3.4, (c) 8.7 and (d) 20 eV. —: present second-order potential model using 16 pseudostates; ---: the 1s-2p close-coupling model of Fon *et al* (1978); - · - · -: the static-exchange model. ●: the data of Williams (1975a, b).

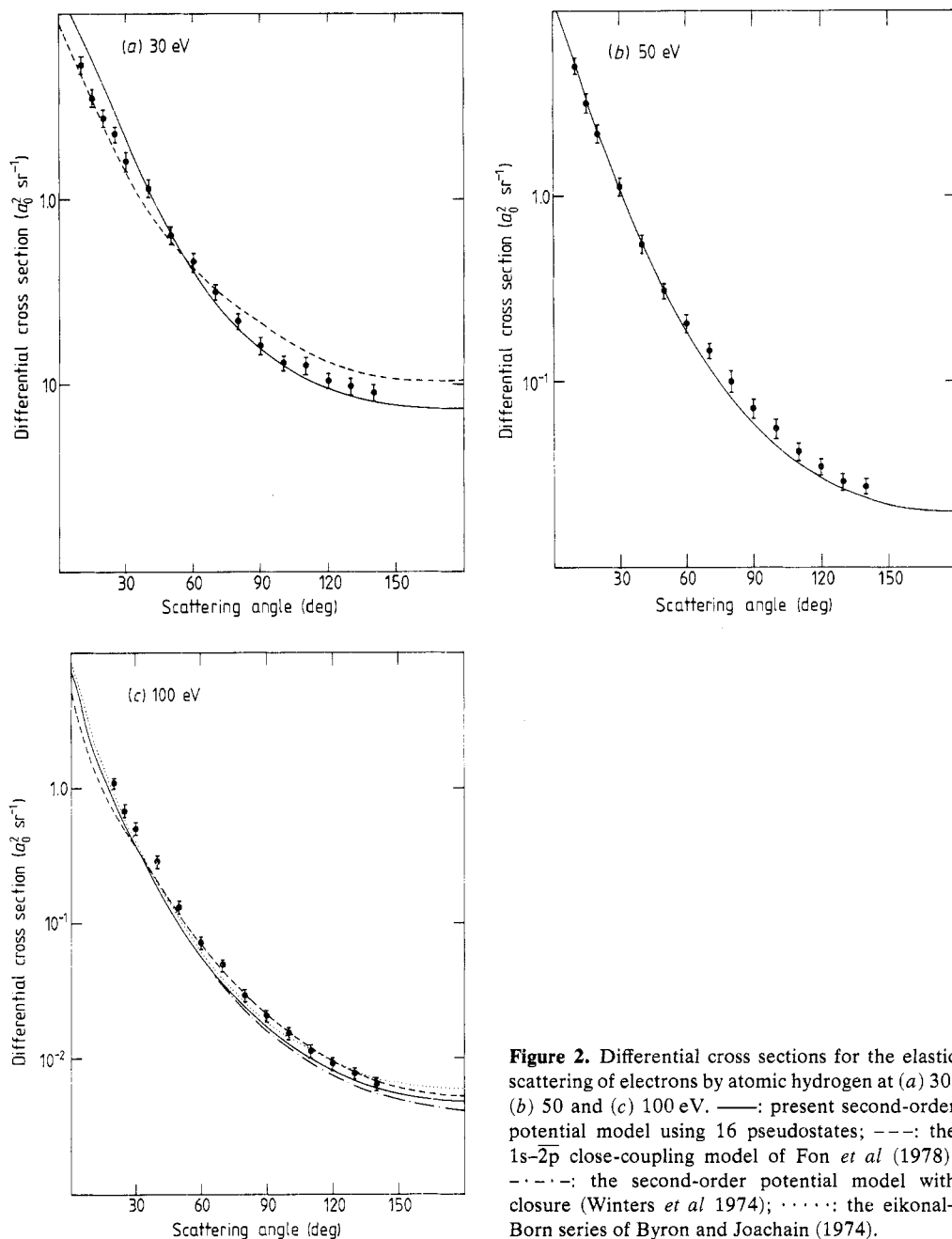


Figure 2. Differential cross sections for the elastic scattering of electrons by atomic hydrogen at (a) 30, (b) 50 and (c) 100 eV. —: present second-order potential model using 16 pseudostates; ---: the $1s\text{--}2p$ close-coupling model of Fon *et al* (1978); - · - · -: the second-order potential model with closure (Winters *et al* 1974); · · · · ·: the eikonal-Born series of Byron and Joachain (1974).

At the three lowest energies Fon *et al* (1978) have calculated a hybrid differential cross section in which the very accurate variational phaseshifts of Schwarz (1961) for $L = 0$, of Armstead (1968) for $L = 1$ and Gailitis (1965) for $L = 2$ are employed together with the phaseshifts from the $1s\text{--}2p$ approximation for $L \geq 3$. These differential cross sections are compared with our own in table 4. At 1.22 eV the agreement is very close. At 3.4 and 8.7 eV the agreement is generally close for $\theta > 60^\circ$, but at smaller angles the

Table 3. Total elastic cross sections in units of πa_0^2 .

E (eV)	σ_{el}
1.22	23.54 23.4
3.4	15.37 15.4
8.7	9.13 9.23

First row: present optical potential model incorporating 16 pseudostates and first-order exchange.

Second row: optical potential model of Coulter and Garrett (1978).

Table 4. Elastic differential cross sections for electron scattering by atomic hydrogen (units of $a_0^2 \text{ sr}^{-1}$).

θ (deg)	$E = 1.22 \text{ eV}$		3.4 eV		8.7 eV	
	A	B	A	B	A	B
0	3.94	4.009	6.24	5.900	10.5	9.244
10	3.93	4.014	5.86	5.053	9.42	7.120
20	3.93	4.079	5.04	4.376	7.27	5.519
30	3.98	4.201	4.25	3.846	5.44	4.309
40	4.12	4.376	3.66	3.449	4.12	3.388
50	4.33	4.602	3.24	3.176	3.10	2.688
60	4.60	4.876	2.98	3.023	2.36	2.164
70	4.94	5.193	2.89	2.985	1.87	1.784
80	5.32	5.545	2.95	3.055	1.56	1.525
90	5.74	5.925	3.14	3.222	1.39	1.366
100	6.19	6.320	3.43	3.467	1.32	1.292
110	6.64	6.719	3.79	3.771	1.31	1.288
120	7.09	7.106	4.19	4.109	1.35	1.336
130	7.50	7.467	4.60	4.455	1.42	1.426
140	7.86	7.787	4.98	4.782	1.49	1.523
150	8.16	8.052	5.31	5.066	1.56	1.626
160	8.37	8.251	5.56	5.285	1.62	1.713
170	8.51	8.373	5.72	5.423	1.64	1.772
180	8.55	8.416	5.77	5.470	1.64	1.792

A: present results.

B: hybrid calculation of Fon *et al* (1978)—see text.

present results exceed those of Fon *et al*, the maximum discrepancy being in the region of 10–20°, where the hybrid calculation agrees better with the data of Williams (1975a).

According to the analysis of experimental data by de Heer *et al* (1977), the maximum of the total (elastic+inelastic) cross sections occurs close to 20 eV and we believe that the large inelasticity of the cross section at 20 and 30 eV is associated with the overestimate of the differential cross section at small angles by our model, in this energy region. To cast light on this, we show in table 5 the computed total elastic and inelastic cross sections compared with the estimates of de Heer *et al*.

Table 5. Total cross sections in units of πa_0^2 .

E (eV)	σ_{el}	σ_{inel}	σ_{tot}
20	4.09	2.23	6.32
	3.35	1.48	4.83
30	2.33	2.65	4.98
	2.01	1.98	3.99
50	1.22	2.56	3.77
	1.00	2.09	3.09
100	0.46	1.87	2.33
	0.60	1.76	2.36

First row: present optical potential model incorporating 16 pseudostates and first-order exchange.

Second row: data of de Heer *et al* (1977).

It is seen that the second-order potential model provides inelastic cross sections which exceed the de Heer *et al* estimates by about 50% at 20 and 30 eV. This suggests that the imaginary part of the potential is too large. Since the comparison of table 2 suggests that the second-order potential represents the inelasticity associated with excitation of discrete levels adequately, we believe that the discrepancy arises from an overestimation of the inelasticity associated with ionisation.

5. Conclusion

We have established that the second-order direct potential for elastic scattering can be constructed from a reasonably small pseudostate basis set. The resulting cross sections agree both with the closure model at high energies and with the results of direct numerical evaluation using exact hydrogenic discrete and continuum functions, at low energies. The agreement with experiment, which is already good at the lowest energy and at 50 eV and above could, in principle, be improved by employing a Hartree-Fock rather than a free-particle Green's function in intermediate states and allowing fully for second-order exchange terms. However a more immediate task is to extend the model by including more than one channel explicitly and calculations are in progress in which the second-order matrix potential connecting the 1s, 2s and 2p channels is constructed from the same pseudostate set employed in this paper.

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