

Electron impact excitation of H and He⁺

I. 1s → ns transitions

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Abstract. A polarized orbital distorted wave model is used to calculate total and differential cross sections for 1s → ns ($n = 2, 3, 4, 5$) electron impact induced transitions in H and He⁺ from threshold to 20 Ryd. The total cross sections for the 1s → 2s transitions are in good agreement with experiment, but cannot in this model show resonances. The differential cross sections at energies above 100 eV agree closely with those of Geltman and Hidalgo. The model reduces to the Born–Oppenheimer ($z = 0$) or CBO I ($z = 0$) when the polarization and static potentials are omitted.

1. Introduction

While it is generally believed that the Born approximation gives an accurate account of total electron impact excitation cross sections at energies many times threshold and that the Coulomb–Born approximation is equally valid for collisions with positive ions (Burgess *et al* 1970), there is less confidence in their predictions for differential cross sections at large angles (Geltman and Hidalgo 1971). At lower energies such methods fail, not only because they are essentially based on a weak perturbation approximation, but because there is no satisfactory method of including exchange consistently with unitarity (Mott and Massey 1965).

The principal theoretical approach to low energy electron impact inelastic collisions is the close-coupling method and its extensions to include correlation and pseudo-states (Burke and Taylor 1969, Geltman and Burke 1970, Burke and Webb 1970). While such methods are useful in predicting the positions and widths of resonances, it is not clear how well they converge to accurate total cross sections when a truncation is employed.

A number of other methods have recently been suggested for predicting cross sections for the intermediate energy region between the range of validity of the Born approximation and close-coupling methods. These include various eikonal approximations (Tai *et al* 1970, Chen *et al* 1972) and a distorted wave approximation based on the polarized orbital approximation of Temkin (Drachman and Temkin 1972), introduced by Lloyd and McDowell (1969).

Temkin's method strictly applies to elastic scattering only, and allows specifically for polarization of the target by the incident electron (position vector r_2). The polarized target function may be specified as the first-order perturbed function if $r_2 > r_1$ (where r_1 is the position vector of the bound electron) but is better obtained from a variational principle simultaneously with the scattering function. This method has been shown to

give accurate results for the elastic scattering of slow electrons by simple atoms and molecules (Drachman and Temkin 1972) and for photoionization of H^- , He, Li^+ (Bell and Kingston 1967a, b, c) and Li (Matese and LaBahn 1969). Here the polarized orbital scattering function obtained for elastic scattering is used to evaluate the matrix element for photoionization even above the inelastic threshold.

Lloyd and McDowell (1969) applied the same method to the $1s \rightarrow 2s$ and $1s \rightarrow 2p$ transitions in atomic hydrogen, solving the elastic scattering problem using the extended polarization approximation of Callaway *et al* (1968), and then using this function to evaluate the T -matrix element for inelastic scattering. Their results were sufficiently promising to warrant further investigation and, in this paper, a simplified version of their model, neglecting distortions other than the dipole component of the polarization potential, is applied to $1s \rightarrow ns$ ($n = 2, 3, 4, 5$) transitions in H and He^+ .

In § 2, we develop the theory, and discuss orthogonalization effects in § 3. The numerical methods employed are outlined in § 4 and the results presented in § 5. Finally, we state our conclusions in § 6.

2. Theory

The cross section for a transition from an initial state i to a final state f of a hydrogenic system of charge Z due to collisions with electrons of initial energy k_i^2 Ryd may be written

$$Q_{if}(k_i^2) = \frac{\mu^2}{2\pi^2} \frac{k_f}{k_i} \int_{-1}^{+1} |T_{if}|^2 d(\cos \theta) \pi a_0^2 \quad (1)$$

where the T -matrix element, T_{if} , which is a function of initial and final wave vectors \mathbf{k}_i and \mathbf{k}_f related by

$$k_i^2 = k_f^2 + \Delta E_{if} \quad \hat{\mathbf{k}}_i \cdot \hat{\mathbf{k}}_f = \cos \theta \quad (2)$$

may be defined as

$$T_{if} = \langle \psi_f | V_f | \Psi_i^+ \rangle \quad (3)$$

in which ψ_f is the unperturbed wavefunction in the final channel, the interaction potential in that channel being V_f , and Ψ_i^+ is the total scattering function in the initial channel. In the case of electron impact with hydrogenic systems when exchange effects are allowed for, this becomes

$$|T_{if}|^2 = \frac{1}{4} \{ |T_{if}^+|^2 + 3|T_{if}^-|^2 \} \quad (4)$$

in which the plus sign refers to the singlet state and the minus sign to the triplet.

Let the incident electron have position vector \mathbf{r}_2 with respect to the nucleus and let \mathbf{r}_1 be that of the initially bound electron. We may write the total hamiltonian as

$$\begin{aligned} H &= -\frac{1}{2}\nabla_1^2 - \frac{1}{2}\nabla_2^2 - \frac{Z}{r_1} - \frac{Z}{r_2} + \frac{1}{r_{12}} \\ &= H_f + V_f \end{aligned} \quad (5)$$

where we have assumed the target nucleus to have infinite mass, and

$$H_f = -\frac{1}{2}\nabla_1^2 - \frac{1}{2}\nabla_2^2 - \frac{Z}{r_1} - \frac{z}{r_2} \quad z = Z - 1 \quad (6)$$

$$V_f = -\frac{1}{r_2} + \frac{1}{r_{12}} \quad (7)$$

in the direct channel. The final unperturbed state of the total system is then

$$\psi_f(1, 2) = \phi_f(Z, 1)\chi_{k_f}(z, 2) \quad (8)$$

where $\chi_{k_f}(z, 2)$ is the outgoing Coulomb wavefunction of an electron in the field of a nucleus of charge z .

We adopt the following approximation for the total scattering function $\Psi_i^{(\pm)}(1, 2)$;

$$\Psi_i^{(\pm)}(1, 2) = (1 \pm P_{12})[\phi_i(Z, 1) + \phi_{\text{pol}}(1, 2)]F^\pm(2) \quad (9)$$

so that $\Psi_i^{(\pm)}$ is represented by a fully antisymmetrized polarized orbital function (Drachman and Temkin 1972). Here, following Lloyd and McDowell (1969), we explicitly include the initial channel only in Ψ_i^+ , but allow implicitly for all other channels through the polarized target function

$$\xi(1, 2) = \phi_i(Z, 1) + \phi_{\text{pol}}(1, 2).$$

We then determine $F^\pm(2)$ by following the original polarized orbital procedure of Temkin and Lamkin (1961). Thus, making a partial wave expansion of F ,

$$F^\pm(2) = k_i^{-1/2} r_2^{-1} \sum_{l=0}^{\infty} (2l+1) i^l \exp[i\{\delta_l^\pm + \eta_l(k_i)\}] u_l^\pm(k_i r_2) P_l(\cos \theta_2) \quad (10)$$

where, for an initial $1s$ state, $u_l^\pm(k_i, r)$ satisfies

$$\left[\frac{d^2}{dr^2} + k_i^2 - \frac{l(l+1)}{r^2} - 2V_{1s,1s}(r) - 2V_{\text{pol}}(r) \right] u_l^\pm(k_i, r) = \pm X_l^\pm(r) r R_{1s}(r) \quad (11)$$

with

$$V_{1s,1s}(r) = -\frac{z}{r} - \left(Z + \frac{1}{r} \right) e^{-2Zr} \quad (12)$$

and

$$V_{\text{pol}}(r) = -\frac{9}{4x^4} [1 - e^{-2x} (1 + 2x + 2x^2 + \frac{4}{3}x^3 + \frac{2}{3}x^4 + \frac{4}{27}x^5)] \quad (13)$$

in which $x = Zr$.

The exchange terms are obtained by neglecting polarization, so that

$$X_l^\pm(r) = (E_{1s} - k_i^2) \delta_{l0} \int_0^\infty R_{1s}(t) u_l^\pm(k_i, t) t dt + \left(\frac{2}{2l+1} \right) \int_0^\infty R_{1s}(t) u_l^\pm(k_i, t) \gamma_l(t, r) t dt \quad (14)$$

and

$$\gamma_l(r, r') = \frac{r'^l}{r^{l+1}}. \quad (15)$$

It follows that our solution for $u_l^\pm(k, r)$ corresponds to the adiabatic exchange approximation as defined by Drachman and Temkin (1972).

We note that this is not quite correct for p-wave scattering (Sloan 1964), but the introduction of the Sloan correction is equivalent to including a velocity dependent potential and earlier work (Lloyd and McDowell 1969) suggests that it made little difference in the applications we have in mind. We solve for $u_l^\pm(k_i, r)$ subject to the boundary conditions

$$u_l^\pm(k_i, 0) = 0 \quad u_l^\pm(k_i, r) \underset{r \rightarrow \infty}{\sim} k_i^{-\frac{1}{2}} \sin(\phi(r) + \delta_l^\pm) \quad (16)$$

$$\phi(r) \underset{r \rightarrow \infty}{\sim} kr - \frac{1}{2}l\pi + \frac{z}{k} \ln 2kr + \eta_l \quad (17)$$

where η_l is the Coulomb phase shift

$$\eta_l(k) = \arg \Gamma\left(l + 1 - \frac{iz}{k}\right). \quad (18)$$

The term involving $(1 \pm P_{12})\phi_{\text{pol}}(1, 2)F^\pm(2)$ in the expression for T_{if} is difficult to handle, and is omitted from the present work. We take account of the polarization distortion of the target in obtaining the scattering function $F^\pm(2)$, but neglect its further effect on the T -matrix element. There is no obvious justification of this additional approximation, but neglecting this term is consistent with our neglect of exchange polarization terms in (11). Thus finally

$$\begin{aligned} T_{if}^\pm &= \langle \psi_f | V_f | (1 \pm P_{12})\phi_f(1)F^\pm(2) \rangle \\ &= 2\pi(f^\pm \pm g^\pm) \end{aligned} \quad (19)$$

with

$$f^\pm(k_i, k_f) = \frac{1}{2\pi} \int dr_1 \int dr_2 \phi_f^*(Z, 1)\chi_{k_f}^*(z, 2) \left(\frac{1}{r_{12}} - \frac{1}{r_2} \right) \phi_i(Z, 1)F^\pm(2) \quad (20)$$

$$g^\pm(k_i, k_f) = \frac{1}{2\pi} \int dr_1 \int dr_2 \phi_f^*(Z, 1)\chi_{k_f}^*(z, 2) \left(\frac{1}{r_{12}} - \frac{1}{r_2} \right) \phi_i(Z, 2)F^\pm(1) \quad (21)$$

which exactly correspond to equations (41) and (42) of Burgess *et al* (1970), and reduce to these if $F^\pm(r)$ is replaced by $\chi_{k_i}(z, r)$. In this notation the cross section is given by their equations (36) and (37).

We are also interested in the differential cross sections, so making the angular momentum expansion (10) we may write

$$T_{if}^\pm = \sum_{l=0}^{\infty} B_l^\pm P_l(\cos \theta) \quad (22)$$

where

$$B_l^\pm = \frac{4\pi}{\sqrt{k_i}} \exp(i\zeta_l^\pm) [(2l+1)I_A \pm I_B \mp \delta_{l0} C I_C] \quad (23)$$

with

$$I_A = \int_0^\infty u_l^\pm(k_i, r) H_l(k_f, r) f_{1s,ns}(r) r dr \quad (24)$$

$$I_B = \int_0^\infty R_{ns}(r) u_l^\pm(k_i, r) g_{1s,l}(r) dr \quad (25)$$

$$I_c = \int_0^\infty R_{ns}(r) u_0^\pm(k_i, r) r \, dr \quad (26)$$

$$C = \frac{2Z^{3/2}}{Z^2 + k_f^2} \left(\frac{2\pi\alpha}{e^{2\pi\alpha} - 1} \right)^{1/2} \exp\left(2\alpha \tan^{-1} \frac{k_f}{Z}\right) \quad (27)$$

$$\alpha = -z/k_f \quad (28)$$

and

$$H_l(k_f r) = G_l(k_f, z, r)/k_f r \quad (29)$$

where $G_l(k_f, z, r)$ is the regular l th order Coulomb function and

$$\zeta_l^\pm = \eta_l(k_i) - \eta_l(k_f) + \delta_l^\pm(k_i). \quad (30)$$

Then the differential cross section $I(\theta)$ is given by

$$I(\theta) = \frac{1}{16\pi^2} \frac{k_f}{k_i} \sum_{l=0}^{\infty} \sum_{\lambda=0}^{\infty} \{ \cos(\zeta_l^+ - \zeta_\lambda^+) B_l^+ B_\lambda^+ + 3 \cos(\zeta_l^- - \zeta_\lambda^-) B_l^- B_\lambda^- \} P_l(\cos \theta) P_\lambda(\cos \theta) \quad (a_0^2/\text{sterad}). \quad (31)$$

The $f_{1s,ns}(r)$ functions are listed in an appendix for $n = 2, 3, 4, 5$, and $g_{1s,ni}(r)$ is given by

$$g_{1s,i}(r) = r \int_0^\infty R_{1s}(t) H_l(k_f t) \gamma_l(r, t) t^2 \, dt \quad (32)$$

its evaluation being discussed in § 4 below.

3. Orthogonalized cross sections

The potential V_f occurring in (3) is arbitrary up to a constant V_0 ($\nabla V_0 \equiv 0$). Thus any theoretical model should ensure that no transitions can be caused by a constant potential. No trouble arises in an exact solution, for then any change in V_f of this nature is compensated for by a change in Ψ_i^+ .

It is well known (Mapleton 1962) that in computing ionization cross sections of complex atoms, in Born's approximation, the wavefunction describing the final state of the target system must be made orthogonal to the target ground state or else a large, energy independent and erroneous cross section is obtained (Williamson and McDowell 1963).

It suffices to ensure in any approximation calculation that

$$t_{if} = \langle \psi_f | \Psi_i^+ \rangle \equiv 0 \quad (33)$$

and in our model this follows automatically if exchange is neglected. At low impact energies when exchange is important it is natural to adjust Ψ_i^+ to satisfy (33) since Ψ_i^+ is never known exactly. This is the procedure adopted in close-coupling approximations where (Burke and Smith 1962) for every target bound state $\phi_{ni}(1)$ included explicitly in the expansion of Ψ_i^+ , the corresponding scattering function $F_{ni}(2)$ is replaced by

$$\bar{F}_{ni}(2) = F_{ni}(2) - \sum_{n'l' \leq ni} \langle \phi_{n'l'} | F_{ni} \rangle \phi_{n'l'}(2)$$

the correction terms vanishing asymptotically.

In our model this leads to difficulties since we then require to solve a different integro-differential equation for each final state. An alternative procedure is to orthogonalize ψ_f . This is also undesirable since while we must necessarily approximate Ψ_i^+ , in the present problem (one-electron target) ψ_f is known exactly. It is of interest nevertheless to examine this alternative procedure; thus we may satisfy (33) by replacing $\chi_{k_f}(z, 2)$ by

$$\bar{\chi}_{k_f}(z, 2) = \chi_{k_f}(z, 2) - \beta \phi_{1s}(Z, 2) \quad (34)$$

where

$$\begin{aligned} \beta &= \langle \chi_{k_f}(z, 2) | \phi_{1s}(Z, 2) \rangle \\ &= \frac{4\pi^{1/2} C e^{-i\eta_0(k_f)}}{Z^2 + k_f^2} \end{aligned} \quad (35)$$

and $\bar{\chi}_{k_f}(z, 2)$ behaves asymptotically as χ_{k_f} .

The modified T -matrix element $T_{if}^\pm(O)$ now becomes

$$T_{if}^\pm(O) = \sum_{l=0}^{\infty} B_l^\pm(0) P_l(\cos \theta) \quad (36)$$

with

$$B_l^\pm(0) = \frac{4\pi}{\sqrt{k_i}} \exp(i\zeta_l^\pm) \{ (2l+1) I_A \pm I_B - \delta_{l0} [E I_E \pm C' I_C \pm D I_D] \} \quad (37)$$

and the additional integrals are

$$I_D = \int_0^\infty R_{ns}(r) u_0^\pm(k_i, r) h_{1s}(r) r \, dr \quad (38)$$

$$I_E = \int_0^\infty R_{1s}(r) u_0^\pm(k_i, r) f_{1s,ns}(r) r \, dr \quad (39)$$

in which

$$h_{1s}(r) = 1 - (1 + Zr) e^{-Zr} \quad (40)$$

and the new coefficients are given by

$$C' = \frac{Z^2 + k_f^2 - 2Z}{Z^2 + k_f^2} C \quad D = E = \frac{2C}{Z^2 + k_f^2}. \quad (41)$$

4. Numerical methods

The work reported in this paper was motivated by a desire to obtain a model which would yield accurate electron impact excitation cross sections at all impact energies for a wide range of transitions of astrophysical interest, and at the same time provide expressions for the cross sections which could be rapidly and cheaply evaluated. The numerical methods adopted appear to meet this criteria, less than fifty seconds central processor time on a CDC 6600 being required for one transition at one energy.

We briefly discuss our methods here, but the program and further details will be reported in a paper to be submitted to *Computer Physics Communications* (Morgan *et al* 1973).

The radial equation (11) for $u_l^\pm(k, r)$ was solved by a non-iterative procedure (cf Marriott and Percival 1958), the normalization and phase shift being obtained by comparison with the JWKB solution (Burgess 1963). The phase shifts are stable to four decimal places and agree well with published values (Drachman and Temkin 1972).

Of the radial integrals involved, only I_C has appreciable long range contributions, its integrand behaving as $(Zr)^n e^{-Zr/n} \sin(kr + \epsilon)$. We found that sufficient accuracy could be attained by using $u_l^\pm(k, r)$ out to $Zr = 14.0$ and then using the Burgess second order JWKB solution to $Zr = 126.0$.

The phase shift difference $\Delta_l = |\delta_l^+ - \delta_l^-|$ decreases rapidly (for fixed k) with increasing l , and we drop the exchange terms in (11) for $l > l_0$ where l_0 is the smallest $l (\neq 0)$ for which Δ_{l_0} is less than 10^{-2} . We replace the non-exchange solution by the appropriate Coulomb or Bessel function for $l > l_1$, where l_1 is the smallest l for which the non-exchange phase shift is less than 10^{-2} . The calculation is terminated when the l th partial cross section changes the total by less than 0.01%.

The Coulomb functions required were generated from the appropriate differential equation by a Numerov procedure, the Bessel functions ($Z = 1$) being treated in the same way, as none of the Library subroutines available were sufficiently rapid.

The function $g_{1s,l}(r)$ was obtained directly from the defining integral rather than by solving the appropriate Hartree differential equation (see McDowell *et al.* 1973).

For $l > l_1$ all integrals except I_A are negligible and I_A reduces to a linear combination of integrals of the form

$$K_{pl}^{(z)}(a, b, c) = \int_0^\infty r^p G_l(ar) G_l(br) e^{-cr} dr \quad p \leq (n-1) \quad (42)$$

where $G_l(ar) = G_l(a, z, r)$ is the regular Coulomb function (or the appropriate spherical Bessel function when $z = 0$). These integrals may be expressed analytically in terms of hypergeometric functions and consequently evaluated much more rapidly than by numerical quadrature.

The Born ($z = 0$) and Coulomb-Born I ($z \neq 0$) cross sections can be obtained directly in terms of these integrals (42) and the published results in these approximations provided a check on the analytic formulation.

We found that for the range of energies investigated ($k_i^2 \leq 20$ Ryd) it was unnecessary to include partial waves $l > 30$ to obtain differential cross sections in $0 \leq \theta \leq 120^\circ$ accurate to 1% within the model. For $\theta \geq 120^\circ$ we had convergence difficulties with $I(\theta)$ for large k_i^2 , since the contributions from the important B_i^\pm in (31) cancelled to several figures as $P_l(\cos \theta) \rightarrow (-1)^l$.

Our code generates the Born and Born-Oppenheimer approximations for $z = 0$ and the CBI and CBOI approximations (Burgess *et al.* 1970) for $z \neq 0$ by using an appropriate data card. In addition it provides (cf § 3) orthogonalized versions of the Born-Oppenheimer and CBOI approximations, the results of which are discussed below. Where a comparison is possible our results agree exactly in all these approximations with the published values.

5. Total and differential cross sections

5.1. Transitions in atomic hydrogen

Total excitation cross sections for the $n = 2$ and $n = 3$ cross sections at low impact energies are displayed in table 1, where they are compared for ($n = 2$) with the results

Table 1(a). Theoretical cross sections for $e + \text{H}(1s) \rightarrow e + \text{H}(2s)$ (in units of $10^{-2} \pi a_0^2$)

k_i^2	0.76	0.77	0.78	0.80	0.81	0.83	0.85	0.90	0.95	1.0	1.1	1.2	1.5
P(U)	8.53	11.2	12.8	14.3	14.7	14.9	14.7	13.4	12.1	10.9	9.41	8.33	9.17
P(O)	88.0	111.3	122.0	—	123.4	114.8	—	76.1	—	38.5	—	—	—
LMcD—	—	14.2	—	18.4	—	—	19.3	17.9	—	14.4	11.0	—	—
GB	14.6	—	16.0	—	19.2	22.2	—	—	—	—	—	—	—
B	—	11.0	—	16.2	—	—	20.7	23.0	—	24.8	25.1	—	—
BO	—	134.0	—	183.0	—	—	204.0	198.0	—	165.5	130.0	—	—
OCH	—	—	—	—	—	—	—	—	—	1.90	—	—	—

P(U) = Present unorthogonalized results, P(O) = Present orthogonalized results. LMcD = Lloyd and McDowell, GB = Geltman and Burke (1970), B = Born, BO = Born–Oppenheimer, OCH = Ochkur approximation (Rudge 1965).

Table 1(b). Theoretical cross sections for $e + \text{H}(1s) \rightarrow e + \text{H}(3s)$ (in units of $10^{-2} \pi a_0^2$)

k_i^2	0.9	0.95	1.0	1.2	1.5	2.0
P(U)	1.96	3.17	3.02	1.81	1.51	1.77
P(O)	21.8	29.5	23.5	6.04	—	—
C.C.	3.2	—	10.5	—	—	—

As table 1(a), C.C. = 6-state close-coupling (Burke *et al.* 1967).

of some simpler approximations. The orthogonalization procedure discussed in § 3 gave very poor results in this case, but the unorthogonalized results for $n = 2$ compare well with the pseudo-state calculations of Geltman and Burke (1970). The earlier calculations of Lloyd and McDowell (1969) differ from the present ones in that they used the extended polarization approximation of Callaway *et al.* (1968) which includes dynamic distortion terms to obtain $u_i^\pm(k, r)$, while we have used a simpler polarized orbitalequation. Our present results lie some 20% lower. However Lloyd and McDowell reported a very large triplet $l = 2$ phase shift which we do not find in our present calculations, our phase shifts being in close agreement with those of Temkin and Lamkin (1951).

The unorthogonalized results for the $1s \rightarrow 3s$ transitions at low energies shown in table 1b are much smaller than the corresponding 6-state close-coupling results of Burke *et al.* (1967). Again, the effect of this form of orthogonalization is poor.

Our low energy calculations for the $1s \rightarrow 2s$ transition are compared with the pseudo-state calculation of Geltman and Burke (1970) and the experiments of Kaupilla *et al.* (1970) and of Kleinpoppen (Koshmieder *et al.* 1972, private communication 1973) in figure 1. The Kaupilla *et al.* results are obtained relative to the $1s \rightarrow 2p$ measurement of Long *et al.* (1968) normalized to the Born approximation (plus cascade correction) at 200 eV as discussed by Geltman and Burke (1970 p 1068). They are in excellent agreement with our unorthogonalized calculations in this energy range. We have normalized Kleinpoppen's relative measurements to our results at $k_i^2 = 0.8$ Ryd. They appear consistent, with this normalization, with the data of Kaupilla *et al.*, and show some resonance structure with a minimum near $k_i^2 = 0.86$ and a maximum near $k_i^2 = 0.87$, which is not allowed for in our model. It should be noted that they are reported as preliminary values.

Our results for the $1s \rightarrow 2s$ transition at higher energies are shown in figure 2, where they are compared with the Born approximation, the pseudo-state calculation of Burke

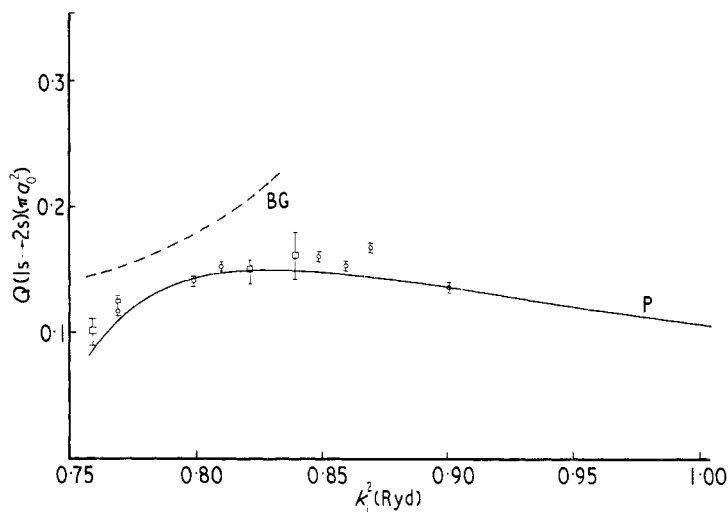


Figure 1. Total cross sections for the process $e + \text{H}(1s) \rightarrow e + \text{H}(2s)$. Present results (P), pseudo-state calculation of Geltman and Burke (1970) (BG). Experimental results of Kaupilla *et al* (1970) are denoted by \bar{Q} , and the relative results of Kleinpoppen (1973) normalized to our value at $k^2 = 0.80$ by \tilde{Q} .

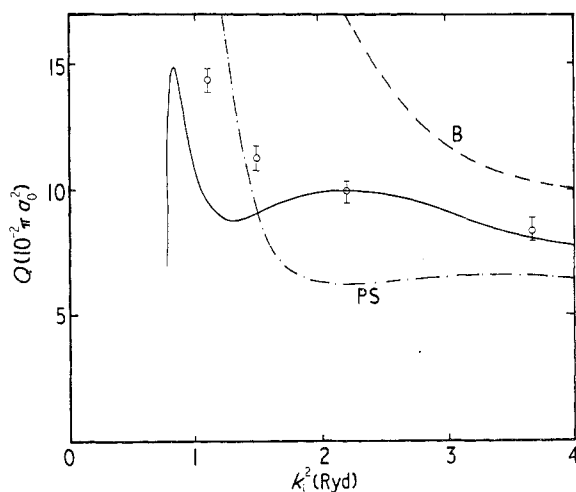


Figure 2. As for figure 1, Present result (P), pseudo-state calculations of Burke and Webb (1971) (PS), Born approximation (B). Experimental results of Kaupilla *et al* (1970) denoted by \bar{Q} .

and Webb (1971) and the experimental data of Kaupilla *et al* (1970). Agreement with experiment is excellent except for the energy range from the resonance region below the $n = 3$ threshold to 1.5 Ryd, and our results go smoothly into the Born approximation at very high energies ($k_1^2 \gg 20$ Ryd). Both the $n = 2$ and $n = 3$ calculations show a secondary maximum, in agreement with the earlier calculation of Lloyd and McDowell (1969).

The calculations have been extended to higher values of n , and the unorthogonalized values for $n = 2, 3, 4, 5$ over a wide range of energies are reported in table 2, since they

Table 2. Total cross section (in units of πa_0^2) for the reaction $e + H(1s) \rightarrow e + H(ns)$ for $n = 2, 3, 4, 5$

k_i^2 (Ryd)	1.0	2.0	3.0	4.0	7.35	9.0	14.70	22.15
E (eV)	17.6	27.2	40.8	54.4	100.0	122.4	200.0	300.0
$n = 2$	1.09, -1	9.99, -2	9.17, -2	7.82, -2	5.01, -2	4.23, -2	2.75, -2	1.89, -2
$n = 3$	3.02, -2	1.77, -2	1.73, -2	1.49, -2	9.71, -3	8.24, -3	5.40, -3	3.71, -3
$n = 4$	1.22, -2	6.32, -3	6.32, -3	5.48, -3	3.57, -3	3.04, -3	2.00, -3	1.38, -3
$n = 5$	5.66, -3	3.01, -3	3.04, -3	2.69, -3	1.72, -3	1.46, -3	9.65, -4	6.65, -4

have important astrophysical applications in studies of the atmospheres of hot stars (Myerscough and Peach 1972). The program may readily be extended to higher n , but the long range nature of the integrands leads to an appreciable loss of accuracy, unless extra time and storage is allocated.

Differential cross sections for the $1s \rightarrow 2s$ and $1s \rightarrow 3s$ transitions at 100 and 200 eV are compared by those given by Geltman and Hidalgo (1971) in the Born and Coulomb-projected Born approximations in table 3, the $1s \rightarrow 2s$ results at 100 eV being shown in more detail in figure 3. As expected, they are very close indeed to the Coulomb-projected Born results by this energy.

Table 3. Differential cross sections $\frac{d\sigma}{d\Omega}(a_0^2)$ for $e + H(1s) \rightarrow e + H(ns)$

	θ°	0	45	90	$\sigma(\text{Total}) \pi a_0^2$
$1s \rightarrow 2s$ 100 eV	P	8.30, -1	1.63, -3	1.98, -4	5.006, -2
	GH	9.10, -1	2.61, -3	2.24, -4	5.32, -2
	B	8.86, -1	1.85, -3	6.70, -6	5.77, -2
$1s \rightarrow 3s$ 100 eV	P	1.12, -1	4.39, -4	4.61, -5	9.706, -3
	GH	1.26, -1	7.13, -4	5.50, -5	1.16, -2
	B	1.21, -1	5.67, -4	2.11, -6	1.15, -2
$1s \rightarrow 2s$ 200 eV	P	9.03, -1	2.31, -4	1.88, -5	2.750, -2
	GH	9.48, -1	3.19, -4	2.74, -5	2.96, -2
	B	9.36, -1	8.54, -5	1.43, -7	2.95, -2
$1s \rightarrow 3s$ 200 eV	P	1.24, -1	5.61, -5	5.15, -6	5.398, -3
	GH	1.30, -1	8.03, -5	6.60, -6	5.91, -3
	B	1.27, -1	2.64, -5	4.39, -8	5.87, -3

P = Polarb

G = Geltman-Hidalgo

B = Born.

5.2. Transitions in He^+

Our results for the $1s \rightarrow 2s$ transitions in He^+ are given in table 4. They show no structure, and rise smoothly from a threshold value of $8.14 \times 10^{-3} \pi a_0^2$ to a maximum of $11.77 \times 10^{-3} \pi a_0^2$ at 5 Ryd. In this case the orthogonalized results are slightly lower at all energies. In table 5 we compare them at selected energies with the CBI, CBOI, CBII and CBOII results of Burgess *et al* (1970). The results for CBI and CBOI obtained from our code agree exactly with those of Burgess *et al*. It is of interest to note that the orthogonalization procedure discussed in § 3 gives a substantial improvement in the Born-Oppenheimer results for the $1s \rightarrow 2s$ transition for $z = 0$ and in the CBOI results

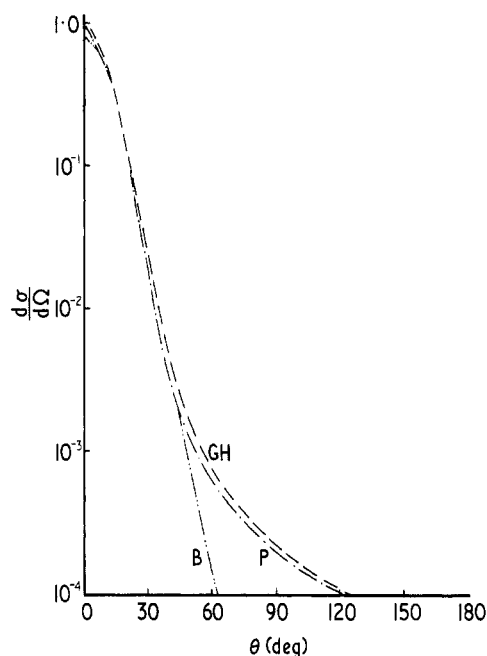


Figure 3. Differential cross sections for $e + H(1s) \rightarrow e + H(2s)$ at 100 eV. B, Born; P, present results; GH, Geltman and Hidalgo (1971) (units of a_0^2/sterad).

Table 4. Total cross sections for $e + He^+(1s) \rightarrow e + He^+(2s)$ (in units of $10^{-3} \pi a_0^2$)

k_i^2 (Ryd)	3.005	3.01	3.04	3.06	3.2	3.3	3.5	3.6	4.0
Q_{1s-2s}	8.16	8.19	8.35	8.45	9.13	9.55	10.26	10.55	11.35
k_i^2 (Ryd)	4.5	5.0	6.0	8.0	10.0	20.0			
Q_{1s-2s}	11.75	11.77	11.23	9.70	8.35	4.79			
<i>Orthogonalized results</i>									
k_i^2	3.005	3.20	10.0	20.0					
$Q_{1s,2s}(O)$	7.63	8.19	8.08	4.77					

Table 5. Comparison of DWPO results with variants of the Coulomb-Born approximation for $e + He^+(1s) \rightarrow e + He^+(2s)$. (Units of $10^{-3} \pi a_0^2$)

k_i^2 (Ryd)	3.0	3.2	3.6	4.0	6.0	8.0
Q	8.14	9.13	10.6	11.4	11.2	9.70
CBOI	85.0	68.8	48.3	36.5	17.1	12.1
CBI	31.4	29.8	27.2	24.8	17.3	13.3
CBII	22.6	17.0	15.1	14.5	12.0	10.1
CBOII	28.7	35.7	24.8	19.0	11.5	9.21

for $z = 1$, (table 6) except at very low energies. Results for higher states follow a similar pattern and are given in table 7, the upper row in each case referring to the unorthogonalized results $Q(U)$, and the lower to the orthogonalized $Q(O)$. The orthogonalized results for $n = 3$ show a secondary maximum.

Table 6. The effect of orthogonalization on the Born–Oppenheimer and CBOI cross sections for the $1s \rightarrow 2s$ transition

	k_i^2 (Ryd)	1.0	2.0	3.0	4.0	9.0	
$z = 0$	B.O.	1.65	2.57, -1	1.32, -1	9.55, -2	4.49, -2	πa_0^2
	B.O.(O)	1.92	1.09, -1	1.05, -1	8.78, -2	4.47, -2	
	k_i^2 (Ryd)	3.2	4.0	6.0	8.0	12.0	
$z = 1$	CBOI	68.8	36.5	17.1	12.1	8.07	$10^{-3} \pi a_0^2$
	CBOI(O)	9.89	13.1	12.9	10.7	7.79	

Note: The second row in each set are the orthogonalized values.

Table 7. Total cross sections for $e + \text{He}^+(1s) \rightarrow e + \text{He}^+(ns)$, ($n = 3, 4, 5$)

	k_i^2 (Ryd)	3.6	3.8	3.9	4.0	5.0	6.0	8.0	10.0	20.0	
$n = 3$	$Q(U)$	1.40	1.54	1.52	1.74	2.11	2.11	1.87	1.61	0.93	$10^{-3} \pi a_0^2$
	$Q(O)$	1.25	1.48	1.46	1.44	1.73	1.81	1.71	1.54	0.93	
$n = 4$	$Q(U)$	—	5.06	5.43	5.76	7.51	7.74	6.88	5.96	3.44	$10^{-4} \pi a_0^2$
	$Q(O)$	—	4.37	4.54	4.72	6.01	6.43	6.22	5.63	3.42	
$n = 5$	$Q(U)$	—	—	2.4	2.6	3.6	3.7	3.3	2.9	1.7	$10^{-4} \pi a_0^2$
	—	—	—	2.1	2.2	2.8	3.1	3.0	2.7	1.7	

There have been two absolute (Dance *et al* 1966, and Peart and Dolder 1973) and one relative (Daly and Powell 1967) measurements of the total cross section for the $1s \rightarrow 2s$ transition in He^+ . While these are consistent in absolute value, (allowing for the lower energy resolution in the experiment of Dance *et al* 1966), they disagree in the magnitude of the observed cross section with the results of a 6-state close-coupling plus correlation calculation of Burke and Taylor (1969) when these are folded with the experimental energy distribution, by almost 50%. Our results, which again cannot show any resonances, are compared with other theoretical results and the experimental results of Peart and Dolder (1973) in figures 4 and 5. The experimental results, which include a cascade contribution are normalized to classically scaled Born calculations (including cascade) at 1 keV.

In figure 5 we compare our results for the $1s \rightarrow 2s$ transition in He^+ , and the same results corrected for cascade, with the experimental points of Dolder and Peart (1972) for the total 2s excitation cross including cascade contributions. To obtain the cascade correction we use classical scaling ($Z^4 Q(Z^2 E) = \text{const}$) to convert the known Born cross sections for $e + \text{H}(1s) \rightarrow e + \text{H}(np)$, $n \leq 6$ and correct for higher p states by an n^{-3} rule. Thus we have

$$\sigma_{\text{cascade}}(1s \rightarrow 2s) = 0.12 \sum_{n \geq 3} \sigma_{np} \quad (43)$$

and allowing for an overestimate of 10% in the n^3 rule for $n \geq 7$,

$$\sum_{n \geq 3} \sigma_{np} \simeq 1.79 \sigma_{3p}$$

giving

$$\sigma_{\text{cascade}}(1s \rightarrow 2s) \simeq 0.215 \sigma_{3p}. \quad (44)$$

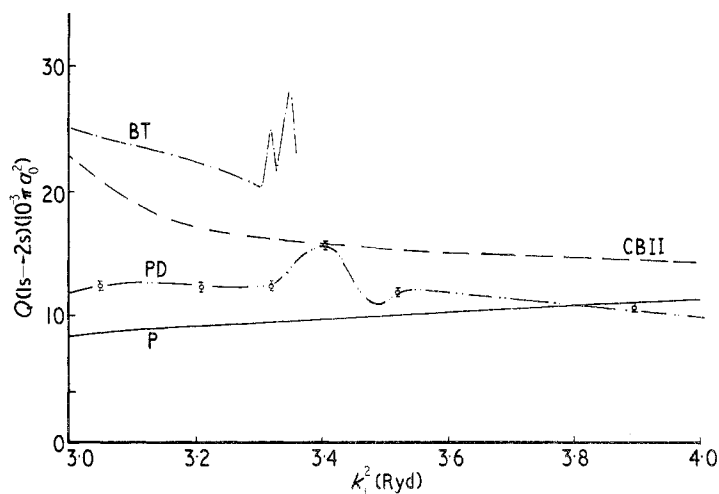


Figure 4. Total cross sections for $e + He^+(1s) \rightarrow e + He^+(2s)$, near threshold. Present results P, Close-coupling plus Correlation (Burke and Taylor 1970) BT, Coulomb Born II (Burgess *et al* 1970) CBII. The dashed curve is drawn through the measured points \bar{Q} of Peart and Dolder (1973).

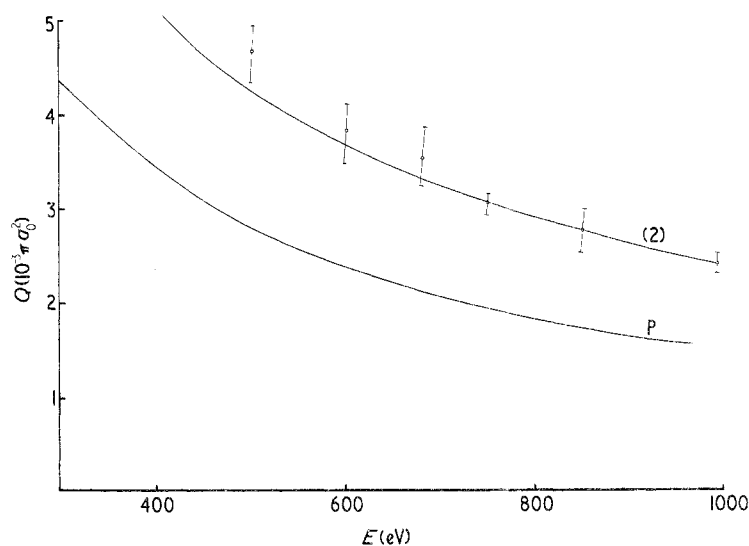


Figure 5. Total cross sections for $e + He^+(1s) \rightarrow e + He^+(2s)$. Present results (P), Curve (2) present results including cascade correction. The measurements of Peart and Dolder are shown by \bar{Q} , the error bars indicating 90% confidence limits.

For hydrogen we have used the data of Vainstein as given by Moiseiwitsch and Smith (1968), and in particular find (with E in eV), for $E \geq 150$ eV.

$$E\sigma_{3p}(E) = 11.43 \ln E - 10.21 + \frac{8.26}{E} (\pi a_0^2 \text{ eV}). \quad (45)$$

Our total 'observed' 2s cross section is then given by

$$\sigma_{2s} = \sigma_{1s \rightarrow 2s} + \sigma_{\text{cascade}}(1s \rightarrow 2s) \quad (46)$$

and for $E \geq 20$ Ryd our results for helium are well fitted by

$$E\sigma_{1s \rightarrow 2s} = \left(110.3 - \frac{308.0}{E}\right) (\pi a_0^2 \times \text{Ryd} \times 10^{-3}). \quad (47)$$

It will be seen from figure 5 that the predictions of (46) are in agreement with the measurements of Dolder and Peart, taking account of their 90% confidence limits, over the whole range of validity of (45), ie $E \geq 600$ eV for He^+ .

Differential cross sections for the $1s \rightarrow 2s$ and $1s \rightarrow 3s$ transitions in He^+ at several energies are shown in figure 6†. Close to threshold they are symmetric about 90° , the exchange (backward) contribution decreasing with increasing energy, until by $k_i^2 = 20$

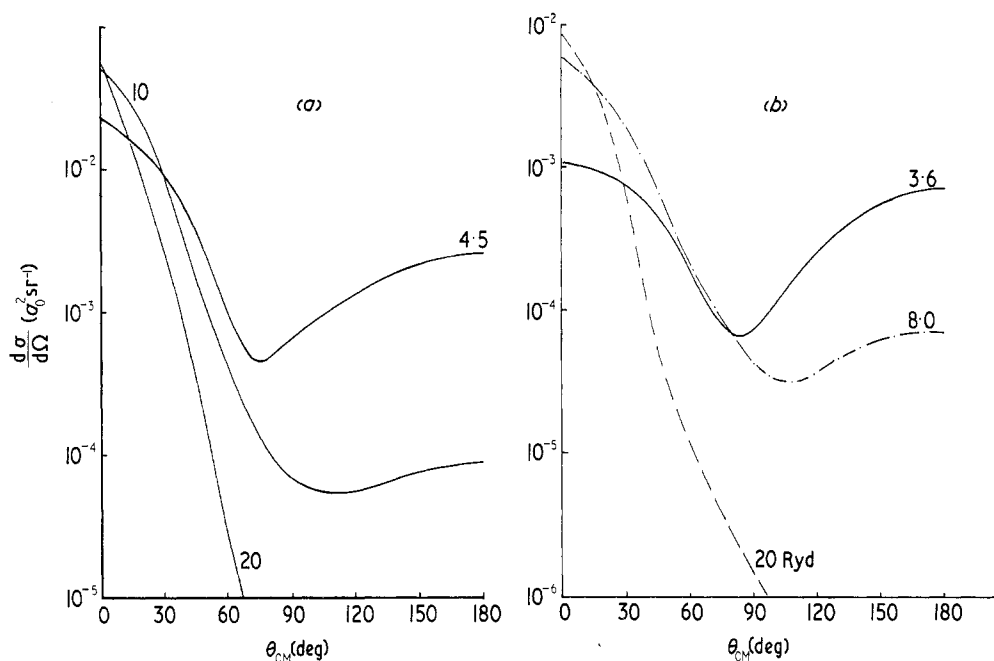


Figure 6. Differential cross sections for (a) the $1s \rightarrow 2s$ and (b) $1s \rightarrow 3s$ transition in He^+ at various energies (k_i^2 Ryd) marked on the curves, in our model, with orthogonalization.

the differential cross section is close to the Coulomb-Born form. The effect of the polarization distortion is quite marked as may be seen from figure 7, where we compare the differential cross section for the $1s \rightarrow 2s$ transition in He^+ at $k_i^2 = 8.0$ Ryd calculated in our model and in the CBOI approximation in which the symmetry about 90° is much more marked.

† The orthogonalized results are shown. The unorthogonalized results, which we now think preferable, are slightly lower at small energies and large angles. They may be obtained by running the published program.

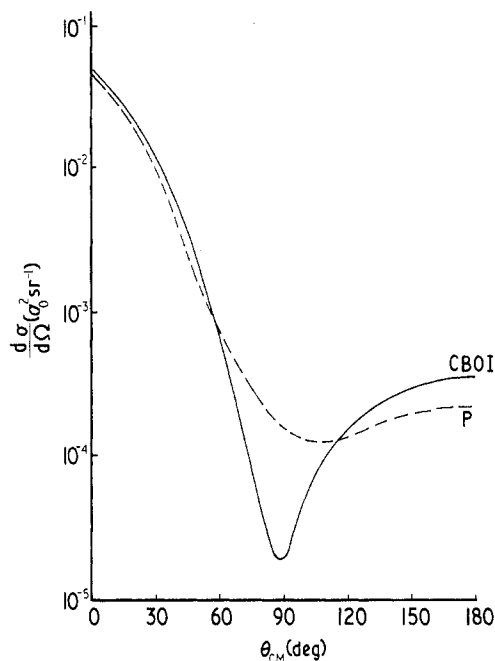


Figure 7. Differential cross sections for $e + He^+(1s) \rightarrow e + He^+(2s)$ at $k_i^2 = 8.0$ Ryd in our model (P) and the CBOI approximation, both orthogonalized.

6. Conclusions

We have shown that the distorted wave polarized orbital approximation provides a useful extension of Born and Coulomb–Born methods for electron impact of one-electron systems, and gives good agreement with experiment (where available) over a wide range of energies. In particular, although the method does not produce resonances, it gives excellent agreement with the measured $1s \rightarrow 2s$ total cross sections both close to threshold and at high energies.

A programme written to evaluate the cross sections and to be submitted to Computer Physics Communications allows rapid evaluation of these DWPO total and differential cross sections, in both orthogonalized and unorthogonalized form, as well as corresponding Born, Born–Oppenheimer, CBI and CBOI results for all z and all energies for $1s \rightarrow ns$ ($n = 2, 3, 4, 5$) transitions in one-electron systems (McDowell *et al* 1973).

The orthogonalization technique reported here is not uniformly successful, and we believe our unorthogonalized results to be more accurate.

The low energy differential cross sections near 90° for $e - He^+ 1s \rightarrow 2s$ and $1s \rightarrow 3s$ transitions are very sensitive to the polarization distortion and may provide an alternative method of measuring polarizabilities of positive ions.

Extensions of this work to $1s \rightarrow np$ and general $nl \rightarrow n'l'$ transitions in one-electron and two-electron systems are in progress and will be reported on in later papers.

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Appendix

The $f_{1s,ns}(r)$ functions which appear in I_A .

$$\begin{aligned}
 f_{1s,2s} &= \frac{4Z}{9\sqrt{2}}(x + \frac{2}{3})e^{-3k/2}, \quad x = Zr \\
 f_{1s,3s} &= \frac{Z}{144\sqrt{3}}(27 + 36x - 8x^2)e^{-4x/3} \\
 f_{1s,4s} &= \frac{Z}{16 \times 24} \left(\frac{81 \times 4^5}{5^5} + \frac{81 \times 4^4}{5^4}x - \frac{22 \times 4^3}{5^3}x^2 + \frac{4^2}{5^2}x^3 \right) e^{-5x/4} \\
 f_{1s,5s} &= \frac{4Z}{5^5 \times 15 \times \sqrt{5}} \left(\frac{5^7 \times 2^7}{6^5} + \frac{5^6 \times 2^7}{6^4}x - \frac{5^4 \times 220}{6^3}x^2 \right. \\
 &\quad \left. + \frac{5^3 \times 100}{6^3}x^3 - \frac{2 \times 5^2}{6^2}x^4 \right) e^{-6x/5}
 \end{aligned}$$

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