Electron impact excitation of atomic hydrogen and hydrogenic ions

B H Bransden† and C J Noble

School of Physical Sciences. The Flinders University of South Australia, Bedford Park, 5042 South Australia, Australia

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Abstract. The second-order potential model of Bransden and Coleman is used to calculate total cross sections for the excitation of the n=2 levels of one-electron ions in the energy interval $25Z^2-250Z^2$ eV, enabling the range of validity of the Coulomb-Born approximation to be assessed. Previously reported work on the excitation of hydrogen is corrected and extended by the inclusion of exchange effects. Good agreement is obtained with the available experimental data.

1. Introduction

The theory of the excitation of one-electron ions has received a good deal of attention, because the cross sections are required for applications in astrophysics and in plasma physics. The most extensive calculations have been in the Coulomb-Born or the Coulomb-Born-Oppenheimer approximations (Burgess *et al* 1970, Jacobs 1971, Tully 1973) and it is important to establish the energy interval for which such methods can be expected to be accurate. The relativistic corrections to these calculations have been examined by Walker (1974). These corrections are negligible for small Z, the nuclear charge, but are of the order of 10% for Z=25, thereafter rapidly increasing with increasing Z. In the non-relativistic regime, 2 < Z < 25, corrections to the Coulomb-Born approximation will be significant for energies close to the excitation thresholds and in fact the measurements of the 1s-2s excitation cross section of He⁺ by Dolder and Peart (1973) show that for this transition, first-order perturbation theory is not accurate until energies above 300 or 400 eV.

For excitation of He⁺, close-coupling calculations in the 1s–2s–2p approximation have been carried out for energies below 218 eV (Burke *et al* 1964, McCarroll 1964). The calculated 1s–2s cross sections disagree badly with the measurements, being a factor of two too large near threshold. This shows that coupling to higher states of the target ion is important. This effect can be taken into account by the second-order potential model of Bransden and Coleman (1972), and in the present work we use this model in a four-state approximation to calculate the excitation cross sections of the 2s and 2p levels of hydrogenic ions for Z=2, 4 and 8 in order to determine at what energies the second-order effects can be ignored. Comparison

[†] Permanent address: Department of Physics, The University of Durham, Durham, England.

is also made with the results of a calculation of the n=2 excitation of He⁺ in the distorted-wave polarized-orbital (DWPO) model by McDowell and co-workers (Lloyd and McDowell 1969, McDowell *et al* 1973, 1974, 1975) which takes into account the real part of the second-order potential, but excludes absorptive effects.

In the third paper of the series by Bransden and co-workers (Sullivan *et al* 1972, to be referred to as III), cross sections were presented for the excitation of the n=2 levels of atomic hydrogen using the second-order potential model in a four-channel $(1s-2s-2p_0-2p_{\pm 1})$ approximation. At the lower energies, these results were inaccurate because of an error in the evaluation of the second-order kernel connecting the s and p levels. In this paper the opportunity is taken to correct these results and to extend them by including the effects of exchange. It should be emphasized that the error in the 2p kernel does not enter into the calculations reported in any of the other papers of the series.

2. Theory

Since in this paper we are primarily interested in scattering at high energies, $(E \ge 100 \, \text{eV})$, we employ the impact-parameter formulation of the second-order potential method described in detail by Bransden and Coleman (1972) and Bransden et al (1972) (to be referred to as I and II, respectively), modified by the inclusion of exchange and Coulomb potentials. In addition, some allowance is made for the differing velocities of the scattered electron in each channel, along the lines suggested by Flannery and McCann (1974a, b).

To introduce the modifications, we expand the total wavefunction of the electronion system in terms of the eigenfunction of the ion, $\phi_n(r)$, to obtain the coupled equations (in atomic units)

$$\left(\nabla^2 + k_n^2 + \frac{2(Z-1)}{r}\right) F_n^{(s)}(r) = 2 \sum_m \left[V_{nm}(r) F_m^{(s)}(r) + (-1)^s W_{nm} F_m^{(s)}(r) \right]$$
(1)

where $F_m^{(s)}(\mathbf{r})$ is the wavefunction of the scattered electron of momentum k_n in the *n*th channel and s is the total spin.

The direct local potential $V_{nm}(r)$ is defined as a matrix element of the interaction between the incident electron and the target ion, omitting the residual Coulomb interaction, -(Z-1)/r, which is included on the left-hand side of equation (1):

$$V_{nm}(r) = \int \phi_n^*(x) \left(\frac{1}{|r-x|} - \frac{1}{r} \right) \phi_m(x) \, \mathrm{d}x. \tag{2}$$

The non-local exchange potential W_{nm} is defined as

$$W_{nm}F_m(r) \equiv \int \phi_n^*(x) \frac{1}{|r-x|} \phi_m(r) F_m(x) dx$$
 (3)

where it is assumed that the functions $F_m(x)$ can be determined so as to be orthogonal to the target eigenfunction ϕ_n .

For elastic scattering Furness and McCarthy (1973), following a procedure of Perey and Buck (1962), have shown that the exchange potential W_{00} can be written

as the operator

$$W_{00}F_0(\mathbf{r}) = 4\pi\phi_0^*(\mathbf{r}) \frac{1}{|\nabla_1 + \nabla_2|^2} \phi_0(\mathbf{r}) F_0(\mathbf{r})$$
(4)

where ∇_1 operates on ϕ_0 and ∇_2 on F_0 . For energies above about 50 eV, Furness and McCarthy show that a good approximation can be obtained by neglecting ∇_1 and replacing $-i\nabla_2$ by the local classical momentum of the scattered electron $(k_0^2 - 2V_L)^{\frac{1}{2}}$, where V_L is the local effective potential. The further approximation in which $-i\nabla_2$ is replaced by the high-energy limit $-i\nabla_2 \to k_0$, has been shown by Vanderpoorten (1975) to be quite accurate even at energies as low as 50 eV. It is not necessary to neglect $-i\nabla_1$ completely, and a small improvement can be obtained by the replacement \dagger $-i\nabla_1 \to \chi_1 \to \chi_2 \in \mathbb{R}$. Retaining the static interaction in V_L , we obtain

$$W_{00}(r) = -\frac{4\pi |\phi_0(r)|^2}{k_0^2 - 2V_{00}(r) + 2(Z - 1)/r + |2\epsilon_0|}.$$
 (5)

For many-channel scattering, the generalization of equation (5) that we adopt, which preserves time-reversal invariance, is

$$W_{nm}(r) = -2\pi\phi_n^*(r)\phi_m(r) \times \left(\frac{1}{k_n^2 - 2V_{nn} + 2(Z-1)/r + |2\epsilon_n|} + \frac{1}{k_m^2 - 2V_{mm} + 2(Z-1)/r + |2\epsilon_m|}\right).$$
(6)

2.1. The impact-parameter equations

The semiclassical phase corresponding to the residual Coulomb interaction, -(Z-1)/r, is logarithmically divergent; therefore before taking the semiclassical limit of equation (1), this term is replaced by the cut-off potential

$$V_{c} = \begin{cases} -(Z-1)/r & r < a \\ 0 & r > a. \end{cases}$$
 (7)

As discussed by Glauber (1959), the cut-off only introduces departures from Coulomb scattering at scattering angles $\theta \le 1/k_n a$, and with a suitable choice of a, the error in the computed total cross sections is negligible.

We now express $F_n(r)$ in the form

$$F_n(\mathbf{r}) = f_n(\mathbf{b}, z) \exp(iS_n) \tag{8a}$$

$$S_n(r) = k_n z - \frac{1}{k_n} \int_{-\infty}^{z} V_c(r) dz$$
 (8b)

where (x, y, z) are the components of r, and $b \equiv (x, y)$ is the impact-parameter vector. Inserting equation (8) into equation (1) and making the usual approximation (see I) of neglecting $(\nabla^2 f_n)$, we find the set of coupled equations for the amplitudes $f_n(b, z)$

$$ik_n \frac{\partial f_n(\boldsymbol{b}, z)}{\partial z} = \sum_{m=0}^{\infty} \overline{V}_{nm}(\boldsymbol{b}, z) \exp[i(S_m(\boldsymbol{r}) - S_n(\boldsymbol{r}))] f_m(\boldsymbol{b}, z)$$
(9)

† The retention of the term $\gtrsim 2\epsilon_0$ corresponds to the Rudge-Bely modification of the Ochkur exchange amplitude (Rudge 1973). The connection between W_{00} and the Ochkur amplitude has been discussed by Vanderpoorten (1975). A critical comparison of exchange potentials has been given by Bransden *et al* (1976).

where

$$\bar{V}_{nm}(b,z) \equiv V_{nm}(r) + (-1)^s W_{nm}(r). \tag{10}$$

These equations represent the necessary generalization of equation (1) in II, where the variable t defined by z = vt was used. Taking the first-order approximation to the equations for m > N, and following the steps leading to equation (5) of II (Bransden et al 1972), we obtain in the closure approximation the set of (N + 1) coupled equations:

$$ik_{n} \frac{\partial f_{n}(b, z)}{\partial z} = \sum_{m=0}^{N} \bar{V}_{nm}(b, z) \exp[i(S_{m}(r) - S_{n}(r))] f_{m}(b, z)$$

$$-i \sum_{m=0}^{N} \exp[i(-S_{n}(r) + \bar{S}(r))] \int_{-1}^{1} dt' f_{m}(b, z') K_{nm}(z, z')$$

$$n = 0, 1, 2, \dots, N$$
(11)

where

$$K_{nm}(z, z') = \exp[i(S_m(r') - \bar{S}(r'))] \left(V_{nm}(z, z') - \sum_{j=0}^{N} V_{nj}(z) V_{jm}(z') \right)$$
(12)

and

$$V_{nm}(z,z') = \int dx \frac{\phi_n^*(x)\phi_m(x)}{|r-x||r'-x|}$$
(13)

The exchange-potential terms are omitted in the definition of the second-order kernel K_{nm} since at the energies with which we are concerned, exchange effects, although significant, are not large. The phase factor \bar{S} is defined as in equation (8b), but with an average momentum \bar{k} replacing k_n ; \bar{k} being defined in terms of an average excitation energy $\bar{\epsilon}$, by

$$\bar{k} = \left[k_0^2 + 2(\epsilon_0 - \bar{\epsilon})\right]^{1/2}.\tag{14}$$

The choice of ϵ has been described in II. The present calculations are performed in a four-channel approximation similar to that reported in III, in which the 1s, 2s, $2p_0$ and $2p_{\pm 1}$ channels are retained explicitly, and in this case we take $\epsilon = 0.078$, to ensure the correct long-range behaviour of the real part of the second-order potential in the incident channel.

From the solution of the coupled equation (11), total cross sections are computed using the expression

$$Q_{0n}(k_0) = \frac{k_n}{k_0} \int d^2b |f_n(b, \infty)|^2.$$
 (15)

3. Numerical methods

The major part of the numerical work lies in the evaluation of the kernels K_{nm} . This was carried out following the method of Coleman (1970, 1972) in the extension described by Bransden *et al* (1976). As in the work reported in III, the coupled equations were solved by Hamming's method (Hamming 1962). A particular point of interest, with the extension of the work to higher energies, is that the range of impact parameters required becomes rather large. For example at $k^2 = 50$ (680 eV),

we require b in the range 0 < b < 100, which corresponds to a range of angular momentum $0 < l \le 700$. For large b (and for large z), the only interaction of importance is the $1s \rightarrow 2p_m$ coupling, which is asymptotically of the form

$$V_{18,2p_{\rm m}}(r) = 1.52462 \, \frac{Y_{1,m}(\theta,\phi)}{r^2}. \tag{16}$$

The range of z over which the integro-differential equations must be solved can be greatly reduced by using starting values obtained by integrating the potential (16)

$$f_{2p,m}(b,z) \simeq -\frac{\mathrm{i}}{k_{2p}} \int_{-\infty}^{-\infty} V_{1s,2p}(r) \exp[\mathrm{i}(S_{2p} - S_{1s})] dz.$$
 (17)

For large $+z_1$, a similar correction, also allowing for the long-range (2s-2p) coupling, was employed.

4. Results and discussion

The total cross sections for the (2s) and (2p) excitations of H have been calculated using our model in the energy range $25-680 \,\mathrm{eV}$, and for the excitation of hydrogenic ions in the energy range $25Z^2-250Z^2$ for Z=2, 4 and 8. The results for hydrogen differ from those reported in III, in that allowance is now made for exchange and that a correction has been made in the calculation of the p-wave kernels (see Bransden et al 1976).

4.1. Total cross sections for the (2s) and (2p) excitation of hydrogen

Our results for the 1s-2s and 1s-2p cross sections for the excitation of atomic hydrogen are shown in tables 1 and 2, compared with the results of some other second-order approximations and the first Born approximation. Below 50 eV the accuracy of our results will be increasingly limited by the semiclassical approximation (Bransden and Noble 1976). However it is interesting to compare them with the recent pseudostate calculation of Callaway et al (1975), which overlaps our energy range and which is expected to be rather accurate. For Q(1s-2s) Callaway et al obtain $0.082 \pi a_0^2$ at 26.6 eV and $0.077 \pi a_0^2$ at 30.6 eV while for Q(1s-2p) they obtain $0.758 \pi a_0^2$ and

Table 1. Calculated cross sections for $e + H(1s) \rightarrow e + H(2s)$ (in units of πa_0^2). Q, present results: Q_B . Born approximation; Q_D DWPO II model, DWPO I above 100 eV (McDowell et al 1973, 1974); $Q_{\rm PS}$, pseudostate model (Flannery and McCann 1974); $Q_{\rm RB}$, second-order diagonalization method (Baye and Heenen 1974).

E(eV)	25	30.6	54	100	136	200	300	400	680
Q	0.076	0.057	0.042	0.036	0.031	0.024	0.018	0.0135	0.0085
$\widetilde{Q}_{ m B}$	0.195	0.167	0.103	0.058	0.043	0.0295	0.020	0.015	0.0088
$Q_{\rm D}$	0.088†		0.073	0.050		0.0275	0.019		
2_{PS}		0.095	0.074#	0.048		0.027			
Q_{BH}	—		0.071‡	0.048		0.027		0.014	

[†] At 26.6 eV.

[‡] At 50 eV.

E(eV)	25	30.6	54	100	136	200	300	400	680
Q	0.66	0.78	0.84	0.66	0.58	0.48	0.35	0.265	0.19
Q_{B}	1.32	1.28	1.04	0.75	0.62	0.48	0.36	0.27	0.19
$Q_{\rm D}$	0.91+		0.85	0.66		0.435	_	-	_
Q_{PS}		0.86	0.89‡	0.65		0.46			_
$Q_{\rm BH}$			0.995‡	0.71		0.46		0.29	100700-10

Table 2. Calculated cross sections for $e + H(1s) \rightarrow e + H(2p)$ (in units of πa_0^2). Q_D . DWPO II model (McDowell *et al* 1975); other notation as in table 1.

 $0.832 \, \pi a_0^2$ at the same two energies. Reference to tables 1 and 2 shows that at these low energies our cross sections are slightly smaller by about 10%, while those of the DWPO II method of McDowell *et al* (1973, 1974, 1975), which embodies the non-absorptive second-order effects is correspondingly a little larger than the accurate result.

A general review of the theoretical approximations which have been applied to excitations of hydrogen will be found in McDowell (1975). Second-order effects can be taken into account in a number of ways, including the pseudostate expansion (Flannery and McCann 1974a, b), the distorted-wave polarized-orbital model (Lloyd and McDowell 1969, McDowell et al 1973, 1974, 1975) and the second-order diagonalization method of Baye and Heenen (1974). Both the calculations of Flannery and McCann and that of Baye and Heenen employed a semiclassical formalism and neither made any allowance for exchange effects. The effect of exchange is to lower the total spin-averaged cross sections slightly, but for the excitation cross sections the effect is small, amounting to no more than 10% at 25 eV. Despite this it should be noted that the individual singlet and triplet cross sections differ considerably at low energies, and for the 1s–2s transition the cross sections for the two spin states still differ by 10% at 400 eV.

As can be seen from tables 1 and 2, the general effect of the second-order potential is to depress the cross section below the results of the first Born approximation (and of those of the close-coupling method) at low energies. As the energy is increased, the Born values are approached, the approach being considerably more rapid in the case of the strong 1s-2p transition.

The various higher-order methods provide cross sections which agree quite well for the 1s-2p transition, but the present method produces cross sections for 1s-2s that are considerably lower than the others at energies less than 200 eV. This may be because the coupling of the 2s channel to other channels is allowed for more fully in the present model. It is not easy to make a definitive comparison between the theoretical results and experiment. The experiment of Kauppila *et al* (1970), because of cascading, effectively measured the combination Q(1s-2s) + 0.23 Q(1s-3p) in the energy range up to $1000 \, \text{eV}$. There have been a variety of calculations of Q(1s-3p), which differ widely at energies below $100 \, \text{eV}$. The DWPO II model of McDowell (1975) is in some respects the closest to our own, and provides 1s-3p cross sections in reasonable agreement with the measurement of Mahan (1974) (see Syms *et al* 1975). Adopting these values for Q(1s-3p), we compare our cascade corrected Q(1s-2s) cross section and experiment in figure 1. The agreement between the form of the computed and measured results is very good. The discrepancies, except perhaps at energies less than $100 \, \text{eV}$, are in normalization and may be largely due to the cascade

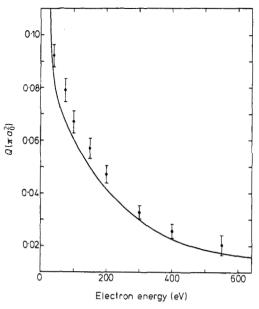


Figure 1. The cross section [Q(1s-2s) + 0.23 Q(1s-3p)] for electron impact excitation of atomic hydrogen. Full curve, the present results; $\overline{\bullet}$, from Kauppila *et al* (1970).

corrections. In this respect it is worth noting that even at $500 \,\text{eV}$ the DWPO II results for Q(1s-3p) are over 10% smaller than those predicted by the Born approximation.

The total cross section for the 1s-2p transition has been measured below 200 eV by Long et al (1968). Our calculated values agree well with the measurements down to 50 eV (see figure 2). It is not surprising that the semiclassical calculation of the (2p) excitation cross section remains accurate at comparatively low energies because the important contributions arise from values of b with b > 1.0, in contrast to the case of (2s) excitations.

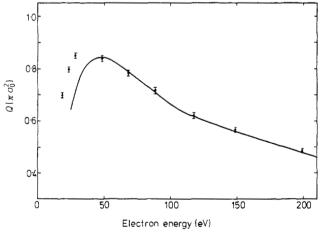


Figure 2. The total cross section for (2p) excitation of atomic hydrogen. Full curve, the present results; ₹, from Long et al (1968).

Table 3. Calculated cross sections for (2s) and (2p) excitation of He ⁻ (in units of πa_0^2).
A, second-order and exchange terms omitted; B, with second-order terms included but
without exchange; C, with both exchange and second-order terms.

E(eV)		Q(2s)		Q(2p)			
	A	В	С	A	В	С	
100	0.0141	0.0070	0.0065	0.117	0.088	0.082	
200	0.0070	0.0053	0.0049	0.074	0.069	0.067	
400	0.0036	0.0032	0.0031	0.049	0.049	0.048	
700	0.0019	0.0020	0.0019	0.034	0.033	0.033	
1000	0.0013	0.0013	0.0013	0.026	0.026	0.026	

4.2. Total cross sections for the (2s) and (2p) excitation of hydrogenic ions

The good agreement obtained with experiment for the n=2 excitation cross sections in hydrogen ensures that the present model is suitable to test the validity of the Coulomb-Born approximation which is used extensively in calculating the corresponding cross sections for electron impact on hydrogenic ions. To demonstrate the magnitude of second-order and exchange effects, cross sections for excitation of He⁺ are shown in table 3 calculated with and without the second-order potential terms and the exchange terms. The reduction in the cross section arising from the second-order potential is seen very clearly at energies below 400 eV, with a further small reduction arising from exchange effects. A similar reduction in cross section is shown in the DWPO model (McDowell et al 1973, 1974, 1975).

The only cross section for Z > 1 which has been measured is for the 1s–2s transition of He⁺ (Dolder and Peart 1973, Dance *et al* 1966). The calculated cross section is compared with that measured by Dolder and Peart in figure 3. The measured cross section has been corrected for cascading and is normalized to the Born approximation at $500 \, \text{eV}$. Both our calculations and those of McDowell *et al* (1973) are in good agreement with the measured values.

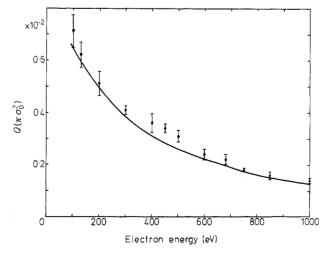


Figure 3. The total cross section for (2s) excitation of He⁺. Full curve, the present results; $\overline{\bullet}$, from Dolder and Peart (1973).

	E(eV)	Z	= 2	4	8	X
$Z^4Q(1s-2s)$	$25Z^{2}$	P	0.10	0.16	0.23	(0.21)+
		CB	0.23	0.24	0.24	0.25
	$50Z^{2}$	P	0.078	0.099		(0.11)
		CB	0.118	0.121	0.12	0.12
	$100Z^{2}$	P	0.050	0.054	0.057	(0.058)
		CB	0.060	0.061	0.061	0.061
	$175Z^{2}$	P	0.030	0.034	Million	(0.034)
		CB	0.034	0.035	0.035	0.035
	$250Z^{2}$	P	0.021	0.024	0.024	(0.024)
		CB	0.024	0.024	0.024	0.024
$Z^4Q(1s-2p)$	$25Z^{2}$	P	1.31	1.42	1.42	(1.42)*
		CB	1.48	1.54	1.57	1.59
	$50Z^{2}$	P	1.07	1.17		(1.09)
		CB	1.10	1.12	1.12	1.13
	$100Z^{2}$	P	0.76	0.77	0.78	(0.75)
		CB	0.75	0.75	0.75	0.76
	$175Z^{2}$	P	0.53	0.52		(0.525)
		CB	0.52	0.52	0.525	0.53
	$250Z^{2}$	P	0.41	0.39	0.39	(0.41)
		CB	0.41	0.41	0.41	0.41

Table 4. Scaled cross sections for n=2 excitation of hydrogenic ions (in units of πa_0^2). P. present results; CB, Coulomb-Born approximation (Tully 1973).

At high energies in the Born approximation, the cross sections for excitation of a discrete level exhibit the scaling law that Z^4Q is a function of $x = Z^2E$. For this reason, we tabulate our computed values of Z^4Q in table 4, together with those of the Coulomb-Born approximation, for energies in the interval $25Z^2-250Z^2$ eV.

For Z > 1, and particularly at the higher energies, very considerable numerical difficulty was experienced in obtaining accurate and stable cross sections. This was especially the case for the (2p) cross sections. The difficulties were associated with evaluating the integrations on the right-hand side of the coupled equations (11) with sufficient accuracy, while keeping the computational time within reasonable bounds. It proved possible to calculate for $Z \le 8$, but for Z = 8 the results were obtained at a more restricted set of energies to conserve computational time. In tables 3 and 4, the (2s) cross sections are considered to be accurate to the figures shown, but the cross sections for (2p) excitation may have errors not exceeding 5%.

The pattern of the results is clear. The cross sections obey the scaling law more and more closely as the energy is increased and the Born approximation is approached, as expected, for large Z and for large E. While, over the energy range considered, the departure of the cross section from the Coulomb-Born approximation value is never very large for the 1s-2p transition, this is not the case for the 1s-2s transition. We have already noticed the big difference between the Coulomb-Born and accurate cross sections for Z=2, and for $E<100Z^2$ the departures are large and significant for Z=4, and for $E<50Z^2$ for Z=8. For large Z the corrections to the Born approximation from exchange effects are relatively of more importance than for small Z, where the second-order potential terms provide the greatest correction.

[†] Coulomb-Born-Oppenheimer approximation (Sampson and Parks 1974).

Table 5. Scaled cross sections for n=2 excitation of He⁻ (in units of πa_0^2). P, present results; CB, Coulomb-Born approximation (Burgess *et al* 1970); CBO, Coulomb-Born-Oppenheimer CBOII approximation (Burgess *et al* 1970).

E(eV)		$Z^4Q(1s-$	-2s)	$Z^4Q(1s-2p)$			
	P	СВ	СВО	P	СВ	СВО	
100	0.10	0.23	0.16	1.31	1.48	1.15	
200	0.078	0.118	0.093	1.07	1.10	1.00	
400	0.050	0.060	0.052	0.76	0.75		

It has been demonstrated by Sampson (1974), that in the limit $Z = \infty$, the Coulomb-Born-Oppenheimer approximation (Burgess *et al* 1970) for electron impact cross sections is exact apart from relativistic corrections. Values for the 1s-2s and 1s-2p cross sections in the $Z = \infty$ limit of this approximation, obtained using the interpolation formulae of Sampson and Parks (1974), are therefore shown in brackets in the last column of table 4.

Coulomb-Born-Oppenheimer (CBO) cross sections for the excitation of hydrogenic ions have been calculated by Burgess *et al* (1970). By interpolating their CBOII results for 1s–2s and 1s–2p excitations of He⁺, which are tabulated for the energy interval from threshold up to 218 eV, we obtain the results shown in table 5. The CBOI results of Burgess *et al* are known to overestimate the L=0 exchange partial cross section for the 1s–2s excitation of He⁺ at low energies, and hence are omitted from table 5. However, it may be noted that in the energy interval between 110 and 220 eV, the CBOI 1s–2s cross section is approximately 9% lower than that of the Coulomb-Born approximation. As shown in table 5, the CBOII cross sections for 1s–2s excitation lie between the Coulomb-Born results and those obtained in the present work. On the other hand, for 1s–2p excitation, our results agree more closely with the Coulomb-Born rather than the CBOII cross sections. This illustrates the possibility, known in other contexts, that Born-Oppenheimer exchange calculations can produce cross sections which are less accurate than those obtained by straightforward use of the Born approximation.

5. Conclusions

The general agreement between cross sections calculated by the present method and the available experiments suggests that the cross sections for excitation of hydrogenic ions given in tables 3 and 4 show the departures from the Coulomb-Born approximation accurately. At all energies these departures are more important for the 1s-2s transition than for the 1s-2p transition. This has the natural explanation that for weak transitions indirect coupling via strongly coupled states is comparatively important compared with direct coupling, while for strong optically allowed transitions only the direct coupling is of importance. It follows that while the Coulomb-Born approximation can be expected to be accurate for the transitions 1s-np, it may be quite inaccurate for many other cases over the energy range considered. This effect has been demonstrated by Bransden and Issa (1975) in their work on the excitation of the n = 3 levels of helium, where it was shown that of the transitions considered the 1s-3d, and to a lesser extent the 1s-3s, cross sections were strongly influenced by indirect coupling even at high energies. In the same way, the departures from

the Coulomb-Born approximation for the excitation of hydrogenic ions would be expected to be more marked for 1s-3s than for 1s-2s and to be even more significant for 1s-3d.

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