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Electron impact excitation of one- and two-electron positive ions

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Abstract. The distorted-wave polarised-orbital (DWPO) model is applied to the evaluation of electron impact excitation cross sections for the lowest $s \rightarrow s$ and $s \rightarrow p$ transitions in one-electron positive ions ($2 \leqslant Z \leqslant 10$) and in helium-like ions ($3 \leqslant Z \leqslant 10$ and Si^{12+}, Ca^{18+} and Fe^{24+}). The results for $He^+(2p)$ are compared with experiment, and the other results with available theoretical models, from excitation threshold to high energies.

1. Introduction

We have applied the distorted-wave polarised-orbital model (McDowell *et al* 1973, 1974, Scott and McDowell 1975, 1976) to calculate excitation from the ground state to the lowest excited s and p states of the one- and two-electron positive ions with nuclear charge $Z \leqslant 10$. We have also carried out calculations for Si^{12+}, Ca^{18+} and Fe^{24+}.

Cross sections for these and similar processes are of fundamental importance in many astrophysical situations (see e.g. Bhatia and Temkin 1977, Seaton 1975), in particular in interpreting the x-ray and EUV spectrum of the solar corona. They are also of great importance both as diagnostic tools and in determining the rates of radiative energy losses in hot plasmas. These applications have been stressed recently by the IAEA Advisory Group on Atomic and Molecular Data for Fusion (McDowell 1977, Hogan 1977).

There is little experimental work, the only results known to us being for $He^+(1s–2s)$ and $He^+(1s–2p)$; the experimental situation has been reviewed recently by Dolder and Peart (1976). Earlier published theoretical work has been reviewed by Seaton (1975). Except for He^+ close to threshold, where close-coupling calculations exist (Burke *et al* 1964, McCarroll 1964, Ormonde *et al* 1967, Burke and Taylor 1969), the theoretical results were then restricted to the Coulomb–Born (CB) approximation and its variants (Burgess *et al* 1970, Tully 1974). Since Seaton's review, Bransden and Noble (1976) have applied the impact-parameter version of Bransden's

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second-order potential method (SOP) to the one-electron sequence. Very recently, Bhatia and Temkin (1977) have carried out distorted-wave calculations for the two-electron sequence, and they and Jones (1974) have also used the University College, London (UCL) distorted-wave code (Eissner and Seaton 1972) to obtain results for comparison. There are also some close-coupling calculations for two-electron ions at low energies (Cooper 1975). Weatherford (1976) has applied a distorted-wave model to the $He^+(1s–2s)$ transition.

The calculations reported here include distorted waves in the initial channel alone, but for two-electron ions, where comparison with the UCL results is possible, they agree closely (see § 3). We include exchange systematically, i.e. both in the distorted wave and in the T matrix. At sufficiently high energies, where distortion is unimportant, our results tend to the Coulomb–Born–Oppenheimer (CBOI) approximation (Burgess *et al* 1970).

Total cross sections for the neutral cases have been reported elsewhere (see Bransden and McDowell 1977 for a review) and are in close agreement with experiment above the first ionisation threshold. We do not anticipate that the present calculations will be sufficiently accurate for all purposes close to threshold, due to neglect of resonance structures.

Our one-electron results are presented in § 2, the two-electron data in § 3 and our conclusions stated in § 4.

2. One-electron ions

We have evaluated cross sections Q for the processes

$$e^- + X^{n+}(1s\,^2S) \rightarrow e^- + X^{n+}(2s\,^2S) \tag{1}$$

$$\rightarrow e^- + X^{n+}(2p\,^2P) \tag{2}$$

without taking account of fine structure, in the DWPO II model (cf Syms *et al* 1975) at selected energies (k_i^2 Ryd) from threshold upwards. Present results are for $2 \leqslant Z \leqslant 10$, though some of the $Z = 2$ results have already been published (McDowell *et al* 1974, 1975). The inelastic differential cross sections for He^+ given in those papers are incorrect, due to an error in sign of a Coulomb phase.

For any isoelectronic sequence it can be shown that $Z^4 E_Z Q(E_Z)$, where $E_Z = (k_i^2/Z^2)$, tends to a finite limit as $Z \rightarrow \infty$ for fixed k_i^2 (Seaton 1975). It is therefore convenient to present results either as scaled cross sections Z^4Q against scaled energy E_Z, or to employ, following Tully (1973), scaled collision strengths Ω'

$$\Omega' = n^3 Z^2 k_i^2 Q = n^3 Z^2 \Omega. \tag{3}$$

Our results for $1s \rightarrow 2s$ transitions are presented in table 1 and for $1s \rightarrow 2p$ in table 2 from threshold to $20Z^2$ Ryd. For $Z = 2$, 4 and 8 comparison with the Coulomb–Born results of Tully (1973) is made in table 3 at three values of E_Z, in terms of scaled cross sections

$$Q' = Z^4 Q(E_Z) = \Omega'/n^3 E_Z \tag{4}$$

all our cross sections being given in units of πa_0^2 ($8{\cdot}797 \times 10^{-17}$ cm^2). In every case the Coulomb–Born–Oppenheimer values (Burgess *et al* 1970) are higher at threshold than the CB results. Table 3 shows that the CB results are always substantially higher

Table 1. Z^4Q for hydrogenic ions: 1s–2s (in units πa_0^2).

E_Z \ Z	1	2	6	7	8	10
0·7501	0·1140, −1	0·1064	0·3701	0·3883	0·4013	0·4190
0·76	0·1061	0·1093	0·3674	0·3850	0·3977	0·4149
0·78	0·1592	0·1148	0·3620	0·3786	0·3907	0·4069
0·80	0·1780	0·1200	0·3567	0·3724	0·3838	0·3992
0·90	0·1639	0·1409	0·3314	0·3436	0·3524	0·3644
1·0	0·1270	0·1538	0·3085	0·3182	0·3254	0·3351
2·0	0·8792, −1	0·1406	0·1791	0·1816	0·1833	0·1860
4·0	0·7323, −1	0·8770, −1	0·9789, −1	0·9842, −1	0·9898, −1	0·9978, −1
6·0	0·5724, −1	0·6324, −1	0·6776, −1	0·6794, −1	0·6820, −1	0·6841, −1
8·0	0·4665, −1	0·4945, −1	0·5182, −1	0·5196, −1	0·5211, −1	0·5227, −1
10·0	0·3928, −1	0·4061, −1	0·4198, −1	0·4210, −1	0·4219, −1	0·4230, −1
15·0	0·2809, −1	0·2806, −1	0·2854, −1	0·2857, −1	0·2865, −1	0·2875, −1
20·0	0·2184, −1	0·2144, −1	0·2165, −1	0·2171, −1	0·2172, −1	0·2180, −1

than our DWPO values. For fixed E_Z this ratio (Q_{CB}/Q_{DWPO}) decreases with increasing Z. The effect of the finite threshold cross section for the positive-ion cases is clearly seen in figures 1 and 2, where we show the 2s and 2p scaled cross sections for $Z = 1$, 2 and 6 as functions of scaled energy E_Z.

We now compare our results with those of Bransden and Noble (1976) in the impact-parameter SOP model. Figure 3 shows our DWPO II results, together with the CB (Tully 1973) and SOP values for excitation of $He^+(1s \rightarrow 2s)$. The SOP results lie lowest, and merge with ours for $E_Z > 7$, while the CB values approach ours from above and are in close agreement by $E_Z > 9$. A comprehensive discussion of the comparison between theory and experiment for this transition has been given by Seaton (1975), the only new calculations since that review being the SOP results and a five-state 1s–2s–2p–$\overline{3s}$–$\overline{3p}$ close-coupling (with $\overline{3s}$, $\overline{3p}$ pseudostates) approach by Henry and Matese (1976). They chose their pseudostates to maximise the overlap with the corresponding (L) continuum. In the energy range where these calculations overlap (100 to 150 eV) the values of Henry and Matese lie above the SOP values and our DWPO II results, but below the CB values, their calculated value of Q' at

Table 2. Z^4Q for hydrogenic ions: 1s–2p (in units πa_0^2).

E_Z \ Z	1	2	6	7	8	10
0·7501	0·7814, −2	1·1209	1·8101	1·8368	1·8562	1·8816
0·76	0·7569, −1	1·1304	1·7941	1·8206	1·8396	1·8650
0·78	0·1262	1·1470	1·7639	1·7911	1·8092	1·8340
0·80	0·1611	1·1606	1·7379	1·7628	1·7818	1·805
0·90	0·3124	1·1976	1·6342	1·6565	1·6724	1·695
1·0	0·4545	1·2086	1·5643	1·5847	1·5987	1·620
2·0	0·9177	1·1541	1·2907	1·3001	1·3070	1·317
4·0	0·8543	0·9421	0·9957	0·9995	1·0023	1·006
6·0	0·7278	0·7782	0·8112	0·8132	0·8151	0·8177
8·0	0·6284	0·6642	0·6882	0·6888	0·6910	0·6930
10·0	0·5533	0·5813	0·6003	0·6017	0·6029	0·6043
15·0	0·4292	0·4480	0·4610	0·4620	0·4628	0·4637
20·0	0·3536	0·3680	0·3780	0·3786	0·3793	0·3801

Table 3. Variation of Z^4Q with E_Z for hydrogenic ions.

		$Z = 2$			$Z = 4$			$Z = 8$		
	E_Z	(a)	(b)	(b)/(a)	(a)	(b)	(b)/(a)	(a)	(b)	(b)/(a)
$1s \rightarrow 2s$	0·75	0·1064	0·5028	4·726	0·3021	0·5330	1·764	0·4013	0·5558	1·385
	1·5	0·1589	0·2773	1·745	0·2102	0·2893	1·376	0·2339	0·2949	1·261
	3·0	0·1075	0·1438	1·338	0·1212	0·1480	1·221	0·1270	0·1498	1·180
$1s \rightarrow 2p$	0·75	1·121	1·653	1·475	1·697	1·998	1·177	1·856	2·155	1·161
	1·5	1·194	1·573	1·317	1·346	1·665	1·237	1·416	1·707	1·206
	3·0	1·047	1·222	1·167	1·106	1·241	1·122	1·135	1·251	1·102

(a) DWPO II.
(b) CB (Tully 1973).

140 eV ($E_Z = 2{\cdot}57$) being about $0{\cdot}218\ \pi a_0^2$, and considerably above the experimental values (normalised at high energies).

Our results for excitation of $He^+(1s \rightarrow 2p)$ are compared with other theoretical values, and with experiment, in figure 4. The CB, SOP and DWPO II values are all consistent with experiment (Daschenko *et al* 1975) (which is normalised to the CB at 217 eV, and carries relatively large statical errors) at energies above 150 eV, the SOP calculation lying between ours and the CB. At lower energies we are in good agreement with the Henry and Matese (1976) five-state calculation, but the experimental data, while not clearly discriminating between the theoretical models, are in closest accord with a three-state 1s–2s–2p close-coupling calculation (Burke *et al* 1964). Further experimental and theoretical work on both these transitions seems desirable.

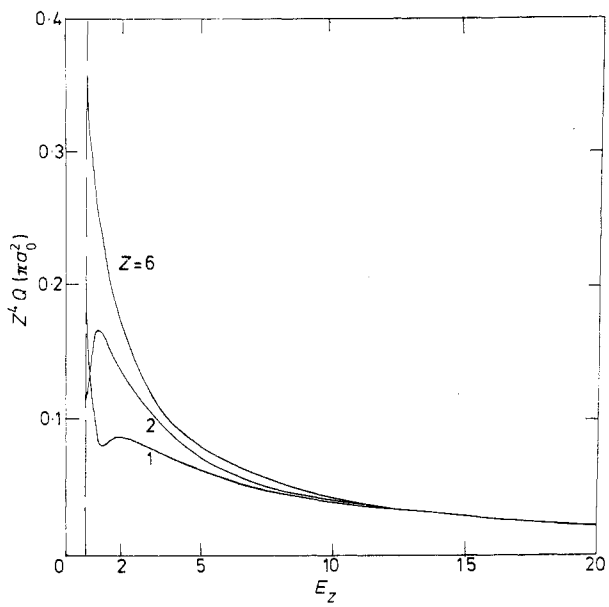

Figure 1. Scaled cross sections Z^4Q (πa_0^2) plotted against scaled impact energies $E_Z = k_f^2/Z^2$ for the $1s \rightarrow 2s$ transition in hydrogenic systems, in the DWPO II approximation. The vertical broken line indicates the excitation threshold.

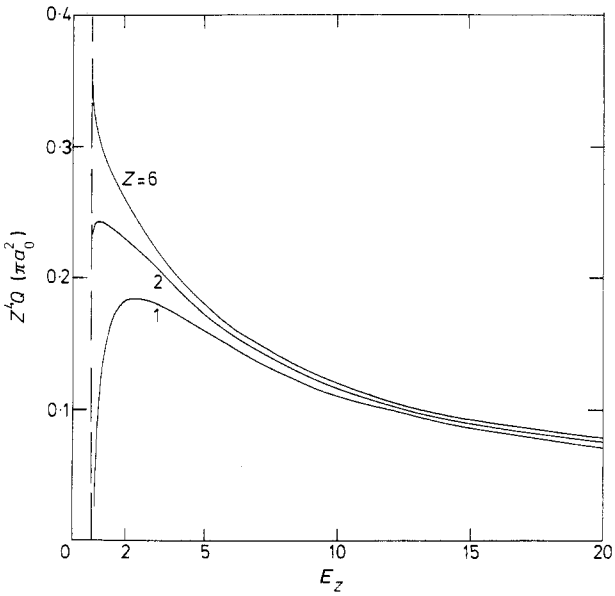

Figure 2. As figure 1 but for the 1s → 2p transition.

3. Two-electron ions

We have evaluated cross sections for the processes

$$e^- + X^{n+}(1s^2\ ^1S) \rightarrow e^- + X^{n+}(1s2s\ ^1S) \tag{5}$$

and

$$e^- + X^{n+}(1s^2\ ^1S) \rightarrow e^- + X^{n+}(1s2p\ ^1P) \tag{6}$$

in the DWPO II model (cf Scott and McDowell (1975, 1976) and Scott (1976) for details of the analysis and numerical methods). Results for $3 \leqslant Z \leqslant 10$ are presented

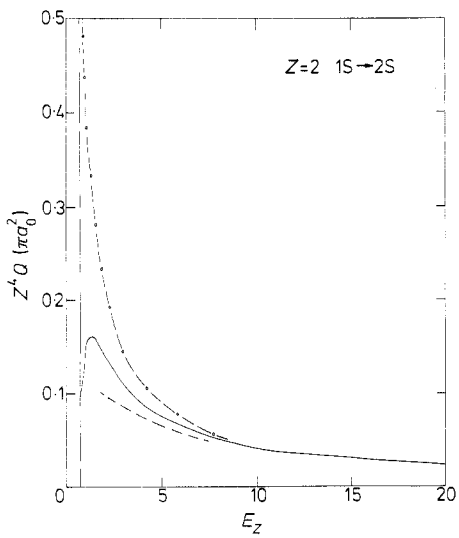

Figure 3. Excitation of $He^-(2s)$: —— DWPO II (this paper); – – – SOP (Bransden and Noble 1976); —·—·— CB (Tully 1973).

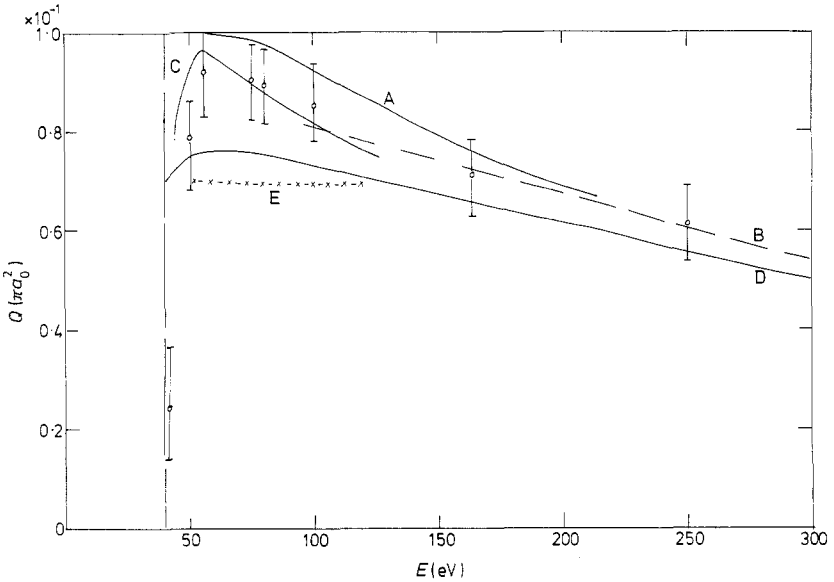

Figure 4. Cross sections for excitation of $He^+(2p)$. Curve A, Coulomb–Born (Tully 1973); curve B, SOP (Bransden and Noble 1976); curve C, 1s–2s–2p CC (Burke *et al* 1964); curve D, DWPO II (this paper); curve E, 1s–2s–2p–$\overline{3s}$–$\overline{3p}$ CC (Henry and Matese 1976). The experimental points (⏀) are due to Daschenko *et al* (1975).

in table 4 for process (5) above, at values of $\epsilon = k_i^2/\Delta E$ between 1 and 10, where ΔE is the threshold energy. Similar results for transition (6) are given in table 5. Results for certain ions with $Z > 10$ are discussed below. Our calculations for helium

Table 4. Cross sections (in units πa_0^2) for excitation of the $1^1S \rightarrow 2^1S$ transition in two-electron ions of charge Z.

ϵ \ Z	3	4	5	6	7	8	9	10
1	4·35, −3	1·12, −3	5·44, −4	3·03, −4	1·60, −4	1·02, −4	6·75, −5	4·63, −5
2	3·63, −3	1·34, −3	5·97, −4	3·03, −4	1·48, −4	8·99, −5	5·77, −5	3·86, −5
3	3·44, −3	1·14, −3	5·07, −4	2·49, −4	1·20, −4	7·19, −5	4·56, −5	3·03, −5
4	3·09, −3	1·03, −3	4·27, −4	2·07, −4	9·90, −5	5·89, −5	3·72, −5	2·46, −5
5	2·74, −3	8·88, −4	3·65, −4	1·75, −4	8·36, −5	4·95, −5	3·12, −5	2·06, −5
10	1·67, −3	5·15, −4	2·07, −4	9·79, −5	4·63, −5	2·73, −5	1·71, −5	1·12, −5

Table 5. Cross sections (in units πa_0^2) for excitation of the $1^1S \rightarrow 2^1P$ transition in two-electron ions of charge Z.

ϵ \ Z	3	4	5	6	7	8	9	10
1	5·951, −3	3·45, −3	1·86, −3	1·04, −3	5·92, −4	3·72, −5	2·44, −4	1·74, −4
2	2·536, −2	9·07, −3	3·91, −3	1·94, −3	1·01, −3	6·01, −4	3·80, −4	7·51, −4
3	2·881, −2	9·62, −3	4·01, −3	1·95, −3	9·97, −4	5·90, −4	3·71, −4	2·44, −4
4	2·809, −2	9·16, −3	3·78, −3	1·82, −3	9·26, −4	5·47, −4	3·43, −4	2·26, −4
5	2·635, −2	8·54, −3	3·50, −3	1·68, −3	8·52, −4	5·03, −4	3·15, −4	2·07, −4
10	1·935, −2	6·15, −3	2·50, −3	1·12, −3	6·02, −4	3·54, −4	2·22, −4	1·46, −4

Table 6. Values of $\Omega' = n^3Z^2\Omega$ for selected Z and ϵ for transitions to 2^1S and 2^1P.

		2^1S			2^1P		
ϵ		$Z = 3$	4	8	$Z = 3$	4	8
1	(a)	1·400	1·282	2·184	1·959	4·015	8·036
	(b)	5·35	5·74	6·42	12·8	16·8	22·6
2	(a)	2·334	3·067	3·850	16·70	21·11	25·96
	(b)	5·94	6·41	6·82	27·5	31·8	37·4
3	(a)	3·318	3·914	4·619	28·46	33·58	38·23
	(b)	6·15	6·58	7·04	37·4	41·9	47·8

(a) DWPO II (this work).
(b) CB (Tully 1974).

(Scott and McDowell 1975, 1976) suggest that our model is unreliable for singlet–triplet transitions at energies below 100 eV. A full discussion is given elsewhere (Bransden and McDowell 1977).

The ground-state wavefunctions used were those of Green *et al* (1954) for $Z \leqslant 6$, of the form

$$\psi(1^1S) = \phi(r_1)\phi(r_2) \tag{7}$$

$$\phi(r) = N(e^{-ar} + ce^{-br}) \tag{8}$$

but for $7 \leqslant Z \leqslant 10$ we used the simpler wavefunctions of Morse *et al* (1935) which take $c = 0$. For the excited states we are grateful to Professor R P McEachran for supplying ten-parameter fixed-core Hartree–Fock functions. This type of function was not employed for the ground state to simplify the solution of the adiabatic exchange scattering equation.

The only previously published calculations of which we know are the Coulomb–Born results of Tully (1974), using Cohen–McEachran functions for both initial and final states. Tully remarks that an earlier calculation by Sural and Sil (1966) is in error, and N C Sil (private communication) agrees (see also Das *et al* 1976, Sil 1977).

The DWPO II results are everywhere smaller than the CB values, and particularly so close to threshold. A comparison of scaled collision strengths Ω' for selected Z and ϵ is given in table 6. The CB results are closest to ours for 2^1P at large Z

Table 7. Coulomb–Born, Coulomb–Born exchange and Coulomb–Born–Oppenheimer cross sections for the $1^1S \rightarrow 2^1S$ transition in two-electron ions (in units πa_0^2).

		CB			CBE	CBO (prior)	CBO (post)
	ϵ	(a)	(b)	(c)	(b)	(c)	(c)
Li^+	1	1·635, −2	1·586, −2	1·328, −2	4·263, −2	3·55, −2	5·92, −2
Be^{2+}	1	5·05, −3	4·97, −3	4·16, −3	7·17, −3	6·69, −3	8·53, −3
	2	2·82, −3	2·78, −3	2·29, −3	2·42, −3	1·98, −3	1·83, −3
	3	1·93, −3	1·89, −3	1·56, −3	1·62, −3	1·33, −3	1·28, −3
	4	1·48, −3	1·43, −3	—	1·25, −3	—	—

(a) Tully (1974).
(b) This work.
(c) Das *et al* (1976).

and ϵ, but our values for $Z = 10$ (not shown) are still much lower than Tully's $Z = \infty$ limiting values (about 20% at $\epsilon = 3$).

More recently, Das *et al* (1976) have calculated CB and Coulomb–Born–Oppenheimer CBO) results for a number of 2^1S cases of interest, using simple final-state functions. However, at $Z = 8$ their CB result at threshold ($1{\cdot}48 \times 10^{-4}\ \pi a_0^2$) differs from that of Tully ($3{\cdot}01 \times 10^{-4}\ \pi a_0^2$), with which we agree, by a factor of two.

We have also computed Coulomb–Born exchange (CBE) results for some 1^1S–2^1S transitions for comparison. The CBE approximation is defined for neutral atoms by Bell *et al* (1966) and does not assume that the target functions satisfy the target Schrödinger equation exactly. Thus it removes the post–prior discrepancy. It may readily be extended to positive ions. Our results are compared with those of Tully (1974) and of Das *et al* (1976, see also Sil 1977) in table 7, for Li^+ and Be^{2+}. The slight differences between our CB results and Tully's at threshold are attributable to our use of the experimental rather than the Hartree–Fock threshold and to the different ground-state function. All three approximations give, as in the one-electron case, much higher values close to threshold than the Coulomb–Born approximation (see also Sampson 1974, Sampson and Parks 1974).

Bhatia and Temkin (1977) have recently applied a distorted-wave model similar to our own to study the same processes. They have also used a distorted-wave code developed at University College, London (Eissner and Seaton 1972) to provide comparison data. (We shall refer to results obtained by Bhatia and Temkin (1977) and Jones (1974) with this code as UCL.)

The distorted-wave approach used by Bhatia and Temkin differs from ours in adopting simpler excited-state functions, and the simpler ground-state function of Morse *et al* (1935) for all Z. They compare their calculated CB values with those of Tully (1974), with which we agree, and find, for example, a value about 16% lower for $Li^+(2^1P)$ at 13·4 Ryd and about 30% lower for $Li^+(2^1S)$ at the same energy. This shows the cross sections are sensitive to the choice of approximate wavefunction, and we regard differences of this order as significant.

We have carefully examined the cross section for the $1^1S \rightarrow 2^1S$ transition in O^{6+} for sensitivity to various changes in the model. We find that although the core polarisation is small ($\alpha_d = 2{\cdot}65 \times 10^{-3}\ a_0^3$ for O^{6+}), results obtained in our model, neglecting polarisation distortion throughout (model (ii)) are some 10% higher for O^{6+} at $\epsilon = 2$ than those given in table 4. The main difference arises in the $l = 0$ contribution. We have examined two further cases: (iii) we replaced the fixed-core Hartree–Fock function for the final state by the three-parameter function of Morse *et al* (1935), and (iv) we modified the single-parameter gound-state function

$$\phi_0(r_1 r_2) = N e^{-\beta(r_1 + r_2)} \qquad (\beta = 7{\cdot}69)$$

by replacing it with the core 1s orbital of the 2^1S function ($\beta = 8{\cdot}0$). The results at $\epsilon = 2$ for 2^1S in O^{6+} are as follows (in units of πa_0^2).

	Q_0	Q_{TOTAL}
(i)	8·4433, −6	8·998, −5
(ii)	1·760, −5	1·023, −4
(iii)	9·341, −8	7·910, −5
(iv)	3·185, −7	6·981, −5

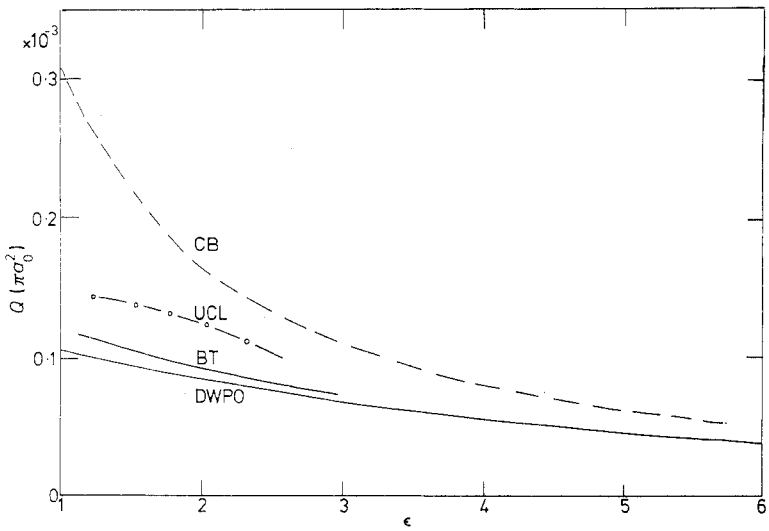

Figure 5. Theoretical results for the cross section for excitation of $O^{6+}(2^1S)$ as a function of ϵ (in units $10^{-3}\ \pi a_0^2$): BT, distorted-wave (Bhatia and Temkin 1977); UCL, see text; CB, Coulomb–Born (Tully 1974 and this work); DWPO, distorted-wave polarised-orbital (this work).

It is clear that even with polarisation distortion omitted the cross section can change by as much as 30% depending on the choice of target wavefunction. Comparing with Bhatia and Temkin's results (for Li^+) we see that inclusion of exchange and distortion by the static potential does not reduce this sensitivity.

In figures 5 and 6 we compare four sets of theoretical results for O^{6+}. For 2^1S (figure 5) our results lie lowest and the Bhatia and Temkin (BT) values lie close to, but above, our results, though they tend to increase more rapidly close to threshold. We estimate that their threshold value is about 20% higher than ours. The values that Bhatia and Temkin obtain with the UCL code are about 50% higher than ours at low energies, but all three sets of results are more than a factor of

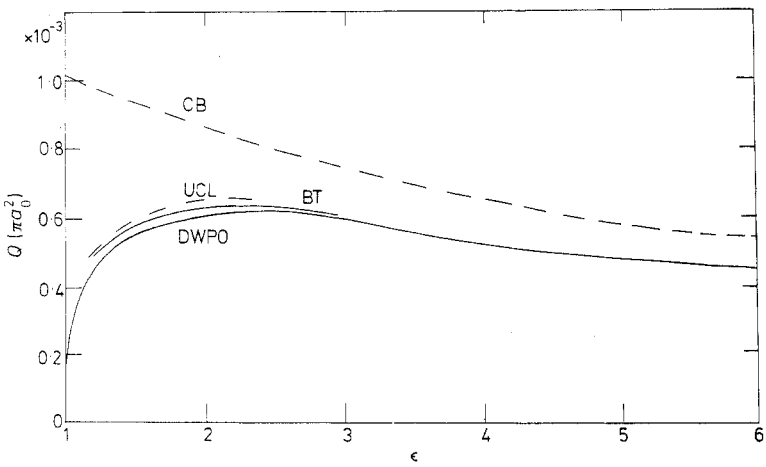

Figure 6. As figure 5 but for $O^{6+}(2^1P)$.

Table 8. Partial-wave contributions to excitation of 2^1P in O^{6+} (in units $10^{-3}\,\pi a_0^2$) for $k_i^2 = 50{\cdot}0$.

l	BT	UCL	DWPO II
0	0·0217	0·0192	0·0194
1	0·0159	0·0104	0·0133
2	0·1588	0·1528	0·1488
3	0·1989	0·2072	0·1870
4	0·0772	0·0792	0·0725
5	0·0188	0·0194	0·0176
6	0·0037	0·0038	0·0035
7	0·0007	0·0007	0·0006
8	0·0001	0·0001	0·0001

For clarification of headings, see text.

two lower than the CB results for $\epsilon < 2$. A similar comparison for $O^{6+}(2^1P)$ is made in figure 6. The partial cross section Q_l ($Q = \Sigma_{l=0}^{\infty} Q_l$) in DWPO II, UCL and BT calculations for $O^{6+}(2^1P)$ at $k_i^2 = 50{\cdot}0$ are shown in table 8. There is close agreement between all three sets of results.

Bhatia and Temkin have also given results for both transitions in Si^{12+}, Ca^{18+} and Fe^{24+}, at several energies. We have modified our codes to use their wavefunctions (which are probably sufficiently accurate for such large Z) and compare our values with their (BT) and Jones' (1974) UCL values in table 9. For both transitions the agreement between the three methods is extremely good. We also show the values computed by Jones using intermediate rather than *LS* coupling. The effects of intermediate coupling are small.

We repeat (Seaton 1975) that none of the calculations reported here can be considered reliable below the first ionisation threshold of the target ion since none incorporate resonance effects, which are known to be of great importance in some cases.

Table 9. Cross sections (in units $10^{-3}\,\pi a_0^2$) for selected high-Z ions.

		k_i^2	(a)	(b)	(c)	(d)
2^1P	Si^{12+}	138	0·0516	0·0502	0·0506	0·051
		196	0·0661	0·0658	0·0668	0·066
	Ca^{18+}	288	0·0103	0·0124	0·0127	0·010
		400	0·0130	0·0154	0·0160	0·013
	Fe^{24+}	493·3	0·00444	0·00432	0·00456	0·0045
		676·0	0·00541	0·00509	0·00559	0·0054
2^1S	Si^{12+}	138	0·014		0·016	0·015
		196	0·013		0·015	0·013
	Ca^{18+}	288	0·0039		0·0040	0·0037
		400	0·0033		0·0037	0·0032
	Fe^{24+}	493·3	0·0013		0·0014	0·0013
		676·0	0·0012		0·0013	0·0012

(a) Bhatia and Temkin (1977).
(b) Jones (1974), intermediate coupling.
(c) Jones (1974), *LS* coupling.
(d) DWPO II.

4. Conclusions

It seems increasingly clear that neither the Coulomb–Born approximation nor any of its variants (Burgess *et al* 1970) are trustworthy for s–s or s–p excitation processes below twice threshold, and may remain poor to quite high energies, especially for s–s transitions, even for Z of order 30. Above this Z, relativistic and spin–orbit effects are important. This conclusion for one- and two-electron systems is reinforced by work on Be^+(2s–2p) for which experimental data are available. This work will be reported elsewhere (Kennedy *et al* 1977, D W Norcross and M Hayes 1977 private communication). The close agreement between our DWPO results, the Bhatia and Temkin results and the UCL values suggest that all are reliable for $\epsilon > 1{\cdot}5$. Astrophysical applications of our results will be reported elsewhere.

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