J. Phys. B: At. Mol. Phys. **15** (1982) 2295–2305. Printed in Great Britain

Electron impact excitation of positive ions in the Coulomb–Born–Bely approximation: calculation for helium-like ions

Shinobu Nakazaki and Tasuke Hashino

Department of Applied Physics, Faculty of Engineering, Miyazaki University, Miyazaki 880, Japan

Received 21 September 1981, in final form 13 April 1982

Abstract. The Coulomb–Born–Bely approximation, which is an extension of the Ochkur–Rudge approximation to the excitation of the positive ion by Bely, has been used to obtain the cross sections for electron impact excitation of helium-like ions ($3 \leq Z \leq 10$, $Z = 14$, 20 and 26). The present cross sections for $1^1S \rightarrow 2^1S$ and $1^1S \rightarrow 2^1P$ transitions have been compared with those of the Coulomb–Born, Coulomb–Born–Oppenheimer and distorted-wave approximations.

1. Introduction

A large number of electron impact excitation cross sections for positive ions are required in order to interpret spectra of astrophysical plasmas and high-temperature laboratory plasmas. Cross sections for excitation from the ground state to the lowest excited s and p states of the one- and two-electron positive ions are of fundamental importance. So far, a lot of work has been done by many theoreticians. The earlier published theoretical work has been reviewed by Seaton (1975). Recently, Henry (1981) has reviewed the theoretical methods and results on the excitation of positive ions by electron impact up to 1980. A simple way of calculating the cross sections for electron impact excitation of positive ions is the Coulomb–Born (CB) approximation. This approximation gives reasonable cross sections for very high incident energies. At low incident energies an effect of electron exchange is important. The Coulomb–Born approximation including the effect of electron exchange is called the Coulomb–Born–Oppenheimer (CBO) approximation.

McDowell *et al* (1977) and Das *et al* (1978) have computed the cross sections for the $1^1S \rightarrow 2^1S$ transition in Li^+ and Be^{2+} by use of the CB and CBO approximations. Their calculated values using the CBO approximation are much higher than their CB results, or the distorted-wave (DW) values of Bhatia and Temkin (1977) and the distorted-wave polarised-orbital (DWPO) results of McDowell *et al* (1977) for near-threshold energies. In C^{4+} the CBO results of Mann (quoted in Magee *et al* 1977) are smaller than his CB results, and are comparable with the DW results of Peek (quoted in Magee *et al* 1977) and the close-coupling (CC) results of Robb (also quoted in Magee *et al*) for low incident energies.

On the other hand, the CBO results for the $1^1S \rightarrow 2^1P$ transition in C^{4+} have been obtained by Mann and are in agreement with the DW results of Bhatia and Temkin (1977) and the CC results of Wyngaarden *et al* (1979). At the present time, it seems that there are no CBO data for other ions in the $1^1S \rightarrow 2^1S$ and $1^1S \rightarrow 2^1P$ transitions.

0022-3700/82/142295+11$02.00

Bely (1966, 1967) has extended the Ochkur (1964) and Rudge (1965) approximations used in the neutral atom to the excitation of positive ions and simplified the exchange scattering amplitude in the CBO approximation. His approximation (the Coulomb–Born–Bely (CBB) approximation) satisfies the orthogonality property of the total wavefunctions before and after the collision, and the detailed balance principle. He has calculated excitation cross sections for the $^3P \rightarrow {}^1D$ transition in the ground configuration of the silicon and carbon series at the threshold excitation energy. He has concluded that his results agree, in general, to within 20 or 30% with those of the exact resonance approximation. Recently, Tully (1980) has applied the CBB approximation to obtain cross sections for some $1^1S \rightarrow n^3L$ transitions in helium-like ions which depend only upon the exchange scattering amplitude. He has concluded that the CBB approximation probably provides a reasonable estimate for excitation of triplet P-state levels but overestimates (underestimates) excitation to n^3S (n^3D) levels by comparison with their Coulomb-projected Coulomb–Oppenheimer results.

The purpose of the present paper is to obtain the cross sections for $1^1S \rightarrow 2^1S$ and $1^1S \rightarrow 2^1P$ transitions in helium-like ions ($3 \leq Z \leq 10$, $Z = 14$, 20 and 26) by use of the CB, CBO and CBB approximations. The present results are compared with those of the DW, DWPO and CC approximations. Atomic units are used unless otherwise stated.

2. Theory and calculations

The differential cross section for excitation from the ground state (α) of a helium-like ion to the singlet discrete state (β) by electron impact in the CBO approximation is given by

$$I(\theta) = (k_\beta / k_\alpha)|f - g^0|^2 \tag{1}$$

where k_α and k_β denote the wavenumber of the incoming and outgoing electrons, respectively, and f and g^0 are the direct and exchange scattering amplitudes, defined as follows

$$f = -\frac{1}{2\pi}\int \Psi_\beta^*(\boldsymbol{r}_1, \boldsymbol{r}_2)\phi_{-k_\beta}(z|\boldsymbol{r}_3)\left(\frac{1}{r_{13}} + \frac{1}{r_{23}} - \frac{2}{r_3}\right)\Psi_\alpha(\boldsymbol{r}_1, \boldsymbol{r}_2)\phi_{k_\alpha}(z|\boldsymbol{r}_3)\,\mathrm{d}\boldsymbol{r}_1\,\mathrm{d}\boldsymbol{r}_2\,\mathrm{d}\boldsymbol{r}_3 \tag{2}$$

$$g^0 = -\frac{1}{2\pi}\int \Psi_\beta^*(\boldsymbol{r}_2, \boldsymbol{r}_3)\phi_{-k_\beta}(z|\boldsymbol{r}_1)(H - E)\Psi_\alpha(\boldsymbol{r}_1, \boldsymbol{r}_2)\phi_{k_\alpha}(z|\boldsymbol{r}_3)\,\mathrm{d}\boldsymbol{r}_1\,\mathrm{d}\boldsymbol{r}_2\,\mathrm{d}\boldsymbol{r}_3. \tag{3}$$

In the above formulae, the functions $\phi_{k_\alpha}(z|\boldsymbol{r})$ and $\phi_{-k_\beta}(z|\boldsymbol{r})$ denote the incoming and outgoing Coulomb wavefunctions corresponding to charge $z = Z - 2$, respectively. The functions $\Psi_\alpha(\boldsymbol{r}_1, \boldsymbol{r}_2)$ and $\Psi_\beta(\boldsymbol{r}_1, \boldsymbol{r}_2)$ are the ground-state and excited-state wavefunctions of target, respectively. The prior and post forms of g^0 are obtained on replacing $H - E$ by

$$\frac{1}{r_{13}} + \frac{1}{r_{23}} - \frac{2}{r_3} \tag{4}$$

and

$$\frac{1}{r_{12}} + \frac{1}{r_{13}} - \frac{2}{r_1} \tag{5}$$

respectively. These simplifications are possible if the wavefunctions Ψ_α satisfy the exact Schrödinger equation for the ion. The post–prior discrepancy arises when approximate wavefunctions are used. Ochkur (1964) and Rudge (1965) have proposed a simple approximation to evaluate the exchange scattering amplitude in the case of scattering by neutral atoms.

Bely (1966, 1967) has extended the procedure suggested by Rudge to the scattering of electrons by positive ions and has presented the simple exchange amplitude which satisfies the principle of detailed balance as follows:

$$g^{\mathrm{B}} = -\frac{2}{k_\alpha^2 + U_\beta} \int \Psi_\beta^*(\boldsymbol{r}_1, \boldsymbol{r}_2)\phi_{-k_\beta}(z|\boldsymbol{r}_2)\Psi_\alpha(\boldsymbol{r}_1, \boldsymbol{r}_2)\phi_{k_\alpha}(z|\boldsymbol{r}_2)\,\mathrm{d}\boldsymbol{r}_1\,\mathrm{d}\boldsymbol{r}_2 \tag{6}$$

where U_β is the ionisation potential of state β. In the CBO approximation the orthogonality condition of the initial and the final wavefunctions is not achieved, while in the CBB approximation the condition is achieved. It also has the advantage that there is no post–prior discrepancy in the CBB approximation.

In order to compare the present CB, CBO and CBB results with the DW results of Bhatia and Temkin (1977) we have used the target wavefunctions of Morse *et al* (1935), which Bhatia and Temkin have employed in their DW calculation.

To evaluate the amplitudes f, g^0 and g^{B} from equations (2), (3) and (6) we use the usual partial-wave expansion. The Coulomb functions $\phi_k(z|\boldsymbol{r})$ may be expanded in terms of partial waves as

$$\phi_k(z|\boldsymbol{r}) = \frac{4\pi}{\sqrt{k}r} \sum_{lm} Y_{lm}^*(\hat{\boldsymbol{k}})\, Y_{lm}(\hat{\boldsymbol{r}})\, \exp(\mathrm{i}\sigma_l(\gamma))\mathrm{i}^l F_{kl}(z|r) \tag{7}$$

with

$$F_{kl}(z|r) = \frac{|\Gamma(l+1-\mathrm{i}\gamma)|}{2\sqrt{k}(2l+1)!} \exp(\tfrac{1}{2}\pi\gamma + \mathrm{i}kr)(2kr)^{l+1}\,{}_1F_1(l+1-\mathrm{i}\gamma; 2l+1; -2\mathrm{i}kr) \tag{8}$$

and $\gamma = z/k$.

Expressing the orbital in the target wavefunction as $\phi_{nl_a}(\boldsymbol{r}) = P_{nl_a}(r)\, Y_{l_a m_a}(\hat{\boldsymbol{r}})/r$, we need to calculate the radial integrals of the following forms to obtain the cross sections.

(i) For the direct amplitude f

$$D_\lambda = \int_0^\infty \int_0^\infty F_{k'l'}(z|r_2)P_{n'l'_a}(r_1)\left(\frac{r_<^\lambda}{r_>^{\lambda+1}} - \frac{\delta_{\lambda_0}}{r_2}\right)F_{kl}(z|r_2)P_{nl_a}(r_1)\,\mathrm{d}r_1\,\mathrm{d}r_2. \tag{9}$$

(ii) For the exchange amplitude g^0

$$E_\lambda^0 = \int_0^\infty \int_0^\infty F_{k'l'}(z|r_2)P_{n'l'_a}(r_1)\left(\frac{r_<^\lambda}{r_>^{\lambda+1}} - \frac{\delta_{\lambda_0}}{r_2}\right)F_{kl}(z|r_1)P_{nl_a}(r_2)\,\mathrm{d}r_1\,\mathrm{d}r_2. \tag{10}$$

(iii) For the exchange amplitude g^{B}

$$E^{\mathrm{B}} = \int_0^\infty F_{k'l'}(z|r)P_{n'l'_a}(r)F_{kl}(z|r)P_{nl_a}(r)r^{-2}\,\mathrm{d}r. \tag{11}$$

These radial integrals are usually evaluated from the Coulomb functions $F_{kl}(z|r)$ ($F_{k'l'}(z|r)$) obtained by numerical integration of the differential equation and atomic radial functions by numerical quadratures. However, the radial integrals D_λ for the monopole ($\lambda = 0$) and dipole ($\lambda = 1$) cases and E^{B} are expressed in terms of the Gauss hypergeometric functions by the method of Nakazaki (1978). The integrals E^{B} in the

CBB approximation may be obtained by using part of the values in the process obtaining the integrals D_λ. Thus, the CBB values can be obtained at the same time as the CB calculation is made. On the other hand, the integrals E_λ^0 in the CBO approximation, which cannot be evaluated analytically, are obtained from the prestored Coulomb functions and atomic radial functions by double numerical quadrature. Therefore, the CBB calculation is very much easier than the CBO calculation.

3. Results and discussions

The detailed computational procedures evaluating the g^0 in the CBO approximation are essentially those described in Burgess *et al* (1970). The radial integrals D_λ and E^B have been calculated using the analytical form. Present cross sections in the CB, CBO and CBB approximations for all energies have been calculated for partial waves $l = 0$–l_{max}. The value l_{max} has been chosen so that the value

$$|Q_l - Q_{l+10}|\left(\sum_{l=0}^{l_{max}} Q_l\right)^{-1}$$

is less than 10^{-6} for large l (Q_l; partial cross sections). In order to check our code we have calculated the cross sections for the $1^1S \rightarrow 2^1S$ transition in Li^+ by use of the CB and CBO approximations using the same target wavefunctions which Das *et al* (1978) have employed in their CB and CBO calculations. The present results in the energy range between threshold and five times the threshold agree to three figures with the CB and CBO results of Das *et al* who have adopted the straightforward method using the numerical integration, without employing partial-wave analysis.

We have calculated the total cross sections for the $1^1S \rightarrow 2^1S$ and $1^1S \rightarrow 2^1P$ transitions in various ions ($3 \leq Z \leq 10$, $Z = 14$, 20 and 26) by use of the CB, CBO and CBB approximations. In the CBO calculation we have obtained the cross sections for the cases of the 'prior' and 'post' forms. Except for ions with small charges near threshold, the post–prior discrepancy was never found to be more than a few per cent. The worse case was found to be in Li^+ for the $1^1S \rightarrow 2^1S$ transition, in which the post and prior forms of the CBO approximation gave results differing by about 30% near threshold.

3.1. The $1^1S \rightarrow 2^1S$ transition

The present total cross sections for the $1^1S \rightarrow 2^1S$ transition in various ions are given in table 1 as a function of the electron energy k^2. In figure 1 the present CB, CBO (prior) and CBB results for the cross section in Li^+ are shown as a function of $X = k^2/\Delta E$, the incident energy in threshold units. At the time the DW results of Bhatia and Temkin (1977), the DWPO results of McDowell *et al* (1977) and the 5CCX results of Wyngaarden *et al* (1979) are shown. The present CBO results are much larger than the CB results, the DW results of Bhatia and Temkin and 5CCX results for $X < 1.5$. In particular, the present CBO results at $X \simeq 1$ are a factor of about ten larger than the present CBB results and the DW results. The 5CCX results of Wyngaarden *et al* are larger by a factor of about five than the CBB results, and the DW results of Bhatia and Temkin. For large $X(\geq 4)$ the 5CCX results are approximately a factor of two larger than the present CB, CBO and CBB results and the DW results of Bhatia

Table 1. Present cross sections for the $1^1S \rightarrow 2^1S$ transition (in units of πa_0^2).

Ion	k^2 (Ryd)	CBO (post)	CBB	Ion	k^2 (Ryd)	CBO (post)	CBB
Li^+	4.373[a]	0.4852−1	0.3023−2	O^{6+}	41.693[a]	0.2111−3	0.1226−3
	4.50	0.4439−1	0.3213−2		50.00	0.1783−3	0.1166−3
	5.00	0.3219−1	0.3740−2		60.00	0.1523−3	0.1103−3
	9.00	0.7753−2	0.4035−2		64.00	0.1442−3	0.1078−3
	13.41	0.4260−2	0.3305−2		75.00	0.1264−3	0.1011−3
	20.00	0.2745−2	0.2501−2		90.00	0.1088−3	0.9233−4
Be^{2+}	8.836[a]	0.7750−2	0.1498−2		105.00	0.9576−4	0.8450−4
	10.00	0.5825−2	0.1553−2		125.20	0.8264−4	0.7545−4
	12.00	0.4007−2	0.1575−2	F^{7+}	53.659[a]	0.1207−3	0.7790−4
	15.00	0.2737−2	0.1518−2		60.00	0.1106−3	0.7548−4
	20.00	0.1857−2	0.1357−2		81.00	0.8819−4	0.6865−4
	25.00	0.1449−2	0.1199−2		100.00	0.7517−4	0.6278−4
B^{3+}	14.801[a]	0.2137−2	0.7084−3		130.00	0.6128−4	0.5450−4
	15.00	0.2086−2	0.7079−3		160.00	0.5181−4	0.4772−4
	18.00	0.1541−2	0.6983−3	Ne^{8+}	67.123[a]	0.7659−4	0.5153−4
	20.00	0.1319−2	0.6874−3		75.00	0.7079−4	0.4987−4
	25.00	0.9893−3	0.6483−3		100.00	0.5773−4	0.4541−4
	27.00	0.9053−3	0.6302−3		150.00	0.4268−4	0.3749−4
	30.00	0.8071−3	0.6025−3		200.00	0.3395−4	0.3130−4
	50.00	0.4928−3	0.4457−3		300.00	0.2411−4	0.2314−4
C^{4+}	22.265[a]	0.8309−3	0.3663−3	Si^{12+}	136.051[a]	0.1896−4	0.1334−4
	25.00	0.7102−3	0.3585−3		138.00	0.1880−4	0.1328−4
	27.00	0.6449−3	0.3531−3		150.00	0.1785−4	0.1292−4
	30.00	0.5698−3	0.3448−3		196.00	0.1496−4	0.1177−4
	36.00	0.4685−3	0.3264−3		300.00	0.1096−4	0.9593−5
	40.00	0.4218−3	0.3134−3		400.00	0.8709−5	0.8002−5
	50.00	0.3421−3	0.2817−3	Ca^{18+}	284.389[a]	0.4355−5	0.3233−5
	60.00	0.2903−3	0.2534−3		288.00	0.4326−5	0.3219−5
	80.00	0.2252−3	0.2086−3		300.00	0.4232−5	0.3175−5
	100.00	0.1849−3	0.1760−3		400.00	0.3569−5	0.2866−5
N^{5+}	31.229[a]	0.3917−3	0.2048−3		500.00	0.3072−5	0.2599−5
	35.00	0.3453−3	0.1992−3		600.00	0.2690−5	0.2362−5
	36.00	0.3352−3	0.1978−3	Fe^{24+}	486.609[a]	0.1477−5	0.1152−5
	40.00	0.3011−3	0.1926−3		493.30	0.1469−5	0.1147−5
	49.00	0.2485−3	0.1808−3		510.00	0.1449−5	0.1134−5
	50.00	0.2440−3	0.1794−3		676.00	0.1254−5	0.1027−5
	60.00	0.2076−3	0.1661−3		750.00	0.1180−5	0.9834−6
	70.00	0.1817−3	0.1535−3		800.00	0.1132−5	0.9555−6
	75.00	0.1713−3	0.1477−3		976.00	0.9898−6	0.8644−6
	80.00	0.1621−3	0.1421−3				

[a] Numbers denote threshold energies ΔE for various ions.

and Temkin. It seems that the cross sections for this transition are sensitive to the choice of approximate wavefunction which is taken for the target. The present CBB results are in agreement within 30% with the DW results and the DWPO results for all incident energies. Figure 2 gives the results for O^{6+}. The present CBB results agree to two figures with the DW results of Bhatia and Temkin (1977) for all values of X. The CB results are larger than the DW and CBO results. The 5CCX results of Wyngaarden *et al* (1979) for $X < 1.5$ lie between the present CBO and CBB results. For $X > 2$ the

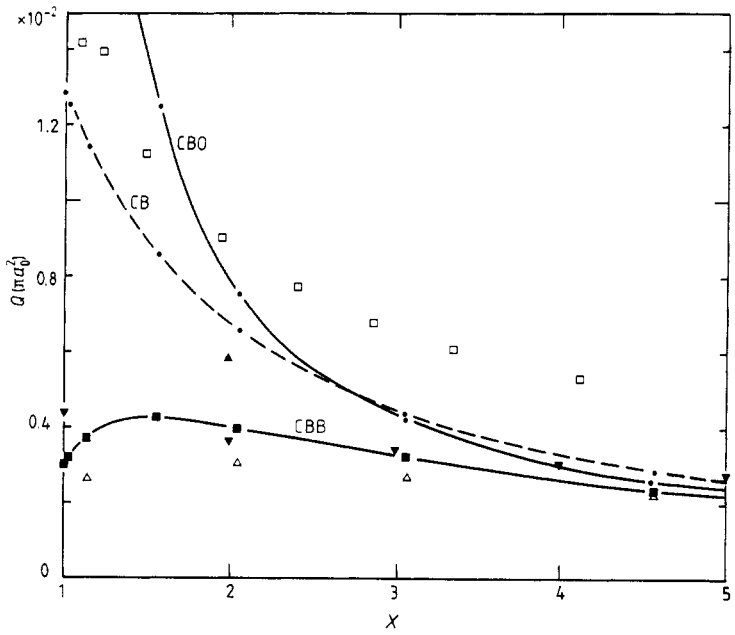

Figure 1. The cross sections for the $1^1S \rightarrow 2^1S$ transition in Li^+ as a function of X (in units of πa_0^2): - - ●- -, present CB results; —●—, present CBO results (prior); —■—, present CBB results; △, DW results of Bhatia and Temkin (1977); ▲, DW results of Baluja and Doyle (1980); ▼, DWPO results of McDowell *et al* (1977); □, 5CCX results of Wyngaarden *et al* (1979).

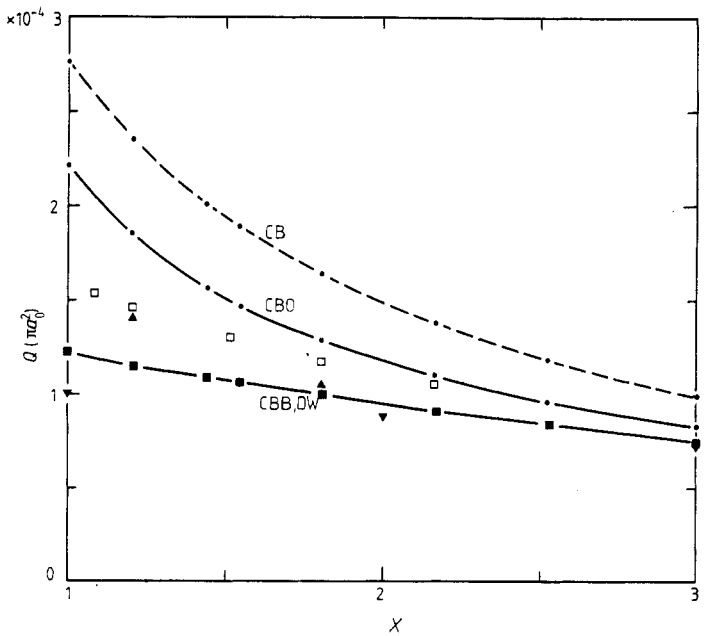

Figure 2. As for figure 1 but for O^{6+}.

CBO results are in close accord with the 5CCX results. Figure 3 gives the results for Si^{12+}. The CB results are approximately a factor of two higher than the CBB, DW and 5CCX results for $X \leq 1.5$. Similar trends are evident for the results made for Ca^{18+} and Fe^{24+}. Agreement between the present CBB results and the DW results of Bhatia and Temkin is best for O^{6+} and the largest discrepancy is for Li^+.

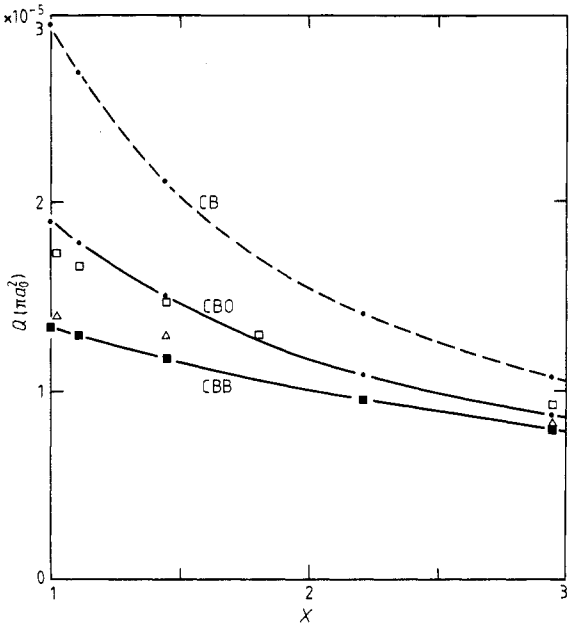

Figure 3. As for figure 1 but for Si^{12+}.

3.2. The $1^1S \rightarrow 2^1P$ transition

In table 2 the present total cross sections for the $1^1S \rightarrow 2^1P$ transition in various ions are listed. Figure 4 compares the present CB, CBO (prior) and CBB results for Li^+ with various results. The 5CCX results of Wyngaarden *et al* (1979) are larger by about 30% than the present CBO results, and the DW results of Bhatia and Temkin (1977) and of Baluja and Doyle (1980) at $X = 1.5$–5. The present CBB results are larger by 75% than the DW results of Bhatia and Temkin at $X \simeq 1$. For $X \geq 2$ differences between the CBB and DW results are within 20%. The CBO results for $X \simeq 1$ are approximately a factor of two higher than the DW results, but for $X \geq 2$ the CBO results are in very close accord with the DW results. Figure 5 gives the results for O^{6+}. Very good agreement exists for the present CBO results with the DW results of Bhatia and Temkin for $X < 3$. The present CB cross sections for partial waves $l = 0$–11 agree to three figures with the results of Bhatia and Temkin for all Z. It seems that their DW results ($l = 0$–11) are lower than the present CBO results ($l = 0$–l_{max}) at $X = 3$ only because the remaining contribution from $l = 12$–∞ is neglected in their calculation. The present CBB results are larger by 35% than the DW results at $X \simeq 1$. For $X \geq 1.5$ the agreement is better than 20%. The 5CCX results of Wyngaarden *et al* lie between the present CBB results and the DW results. For Si^{12+} similar trends are noted to those for O^{6+} (figure 6). The present CBO results are in very good agreement with

Table 2. Present cross sections for the $1^1S \rightarrow 2^1P$ transition (in units of πa_0^2).

Ion	k^2 (Ryd)	CBO (post)	CBB	Ion	k^2 (Ryd)	CBO (post)	CBB
Li^+	4.465[a]	0.2799−1	0.1780−1		64.00	0.5921−3	0.7028−3
	5.00	0.2461−1	0.2177−1		75.00	0.6201−3	0.7067−3
	9.00	0.2722−1	0.3074−1		90.00	0.6323−3	0.6958−3
	10.00	0.2778−1	0.3090−1		105.00	0.6288−3	0.6765−3
	13.41	0.2797−1	0.2992−1		126.30	0.6115−3	0.6446−3
	15.00	0.2756−1	0.2914−1		150.00	0.5858−3	0.6089−3
	20.00	0.2567−1	0.2653−1	F^{7+}	54.081[a]	0.2748−3	0.3885−3
	30.00	0.2180−1	0.2214−1		60.00	0.3070−3	0.4095−3
Be^{2+}	8.983[a]	0.6345−2	0.7611−2		70.00	0.3455−3	0.4309−3
	10.00	0.6830−2	0.8518−2		81.00	0.3716−3	0.4415−3
	12.00	0.7809−2	0.9638−2		100.00	0.3925−3	0.4428−3
	15.00	0.8817−2	0.1036−1		130.00	0.3953−3	0.4268−3
	20.00	0.9464−2	0.1050−1		160.00	0.3837−3	0.4046−3
	25.00	0.9468−2	0.1016−1	Ne^{8+}	67.600[a]	0.1840−3	0.2585−3
	30.00	0.9219−2	0.9702−2		75.00	0.2048−3	0.2717−3
	40.00	0.8510−2	0.8770−2		85.00	0.2254−3	0.2831−3
B^{3+}	15.003[a]	0.2553−2	0.3516−2		100.00	0.2448−3	0.2910−3
	18.00	0.3084−2	0.4006−2		150.00	0.2613−3	0.2849−3
	27.00	0.3869−2	0.4455−2		200.00	0.2521−3	0.2656−3
	40.00	0.3991−2	0.4289−2	Si^{12+}	136.689[a]	0.5217−4	0.7157−4
	50.00	0.3852−2	0.4042−2		138.00	0.5269−4	0.7190−4
C^{4+}	22.523[a]	0.1272−2	0.1807−2		150.00	0.5686−4	0.7442−4
	25.00	0.1436−2	0.1938−2		196.00	0.6633−4	0.7875−4
	27.00	0.1546−2	0.2016−2		300.00	0.7042−4	0.7660−4
	30.00	0.1676−2	0.2097−2		400.00	0.6766−4	0.7121−4
	36.00	0.1843−2	0.2176−2	Ca^{18+}	285.744[a]	0.1029−4	0.1418−4
	40.00	0.1906−2	0.2190−2		288.00	0.1037−4	0.1423−4
	50.00	0.1965−2	0.2160−2		400.00	0.1299−4	0.1552−4
	60.00	0.1950−2	0.2089−2		500.00	0.1379−4	0.1558−4
	80.00	0.1843−2	0.1921−2		600.00	0.1396−4	0.1526−4
	100.00	0.1715−2	0.1763−2	Fe^{24+}	487.915[a]	0.4418−5	0.5957−5
N^{5+}	31.543[a]	0.7112−3	0.1014−2		493.30	0.4463−5	0.5984−5
	36.00	0.8232−3	0.1094−2		510.00	0.4595−5	0.6060−5
	40.00	0.8982−3	0.1140−2		676.00	0.5409−5	0.6427−5
	49.00	0.1003−2	0.1189−2		750.00	0.5580−5	0.6452−5
	60.00	0.1059−2	0.1194−2		800.00	0.5654−5	0.6442−5
	75.00	0.1070−2	0.1161−2		976.00	0.5745−5	0.6310−5
O^{6+}	42.062[a]	0.4296−3	0.6105−3		1500.00	0.5406−5	0.5655−5
	50.00	0.5123−3	0.6647−3		2000.00	0.4932−5	0.5067−5

[a] Numbers denote threshold energies ΔE for various ions.

the DW results of Bhatia and Temkin. The present CB results are larger by a factor of 2.5 than the DW results for $X < 1.2$. It is therefore clear that the effect of electron exchange is important for all Z, and the distortion may be neglected for $X \geqslant 2$. The present CBB results are in agreement within 20% with the DW results for $X \geqslant 2$ for all Z.

To conclude, the CBB approximation involves no more computation than that required by the CB approximation and is quite simple to apply. The CBB approximation removes the defect that the CBO approximation overestimates the cross sections close

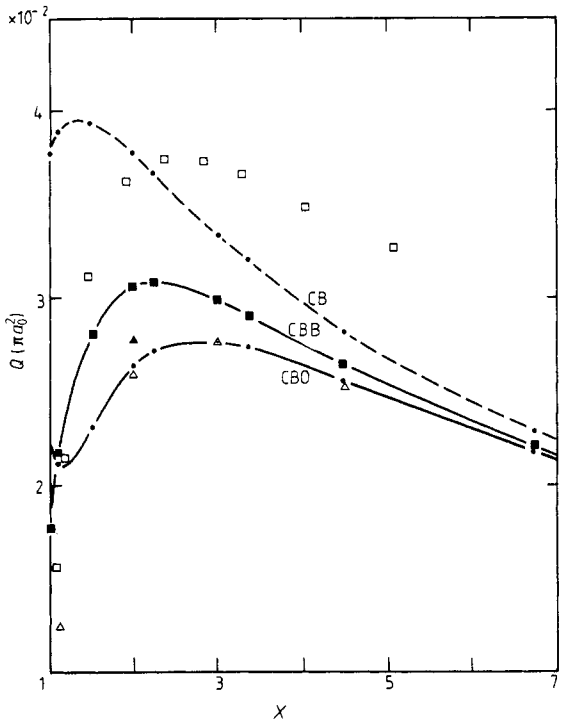

Figure 4. As for figure 1 but for the $1^1S \rightarrow 2^1P$ transition in Li^+.

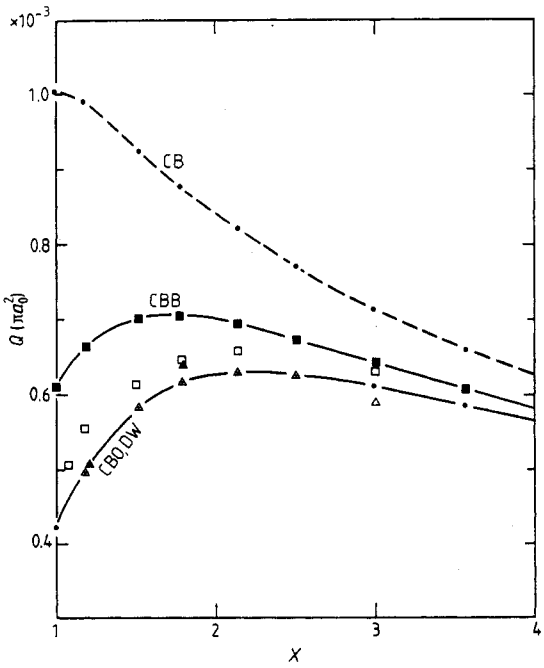

Figure 5. As for figure 1 but for the $1^1S \rightarrow 2^1P$ transition in O^{6+}.

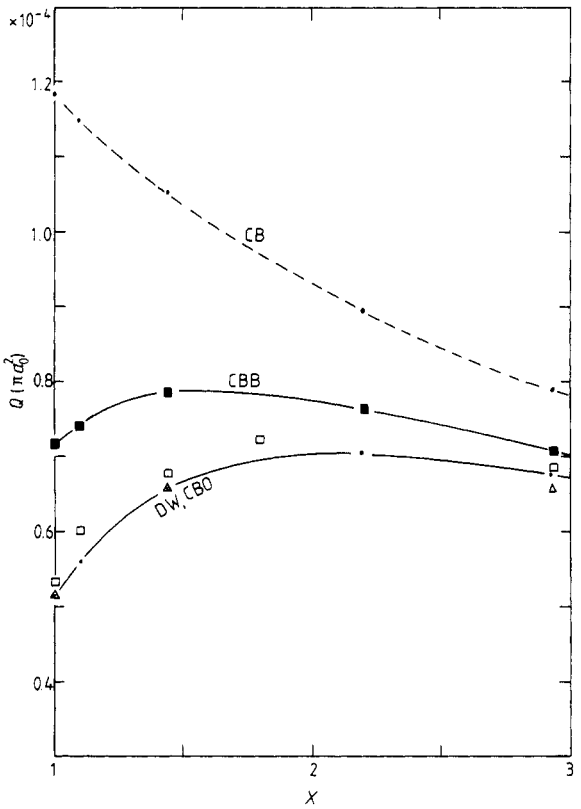

Figure 6. As for figure 1 but for the $1^1S \rightarrow 2^1P$ transition in Si^{12+}.

to threshold for the $1^1S \rightarrow 2^1S$ transition for $Z < 6$. The CBB results for the $1^1S \rightarrow 2^1S$ transition in various ions ($3 \leq Z \leq 10$; $Z = 14, 20$ and 26) agree within 30% with the DW results of Bhatia and Temkin (1977) for $X \simeq 1$. For $X > 2$ the difference between the CBB results and their DW results is within 20%. For the $1^1S \rightarrow 2^1P$ transition the CBO results for all Z are in very good agreement with the DW results of Bhatia and Temkin for all incident energies while the CBB results are larger than their DW results. As Z increases the differences between the present CBB results and their DW results decrease. For both the transitions the CB approximation in general overestimates the cross section. It can be seen from the CBO or DW results that the effect of electron exchange is important even for high incident energies ($X > 3$). It seems that at high incident energies the CBB approximation takes the effect of electron exchange into account well. Although the CBB approximation is for high incident energy, it provides a great improvement over the CB approximation and comparable results with the DW results for the present transitions even for low incident energies. Calculations using the CBB approximation for other transitions are desirable to study the usefulness of this approximation.

Acknowledgments

The authors would like to thank Professor K Takayanagi for initiating interest in this problem. A part of this research has been supported by a Grant in Aid for Scientific

Research from the Ministry of Education, Science and Culture. Numerical calculations have been made on the FACOM M-200 at the Computer Center, Kyushu University.

References

Baluja K L and Doyle J G 1980 *Phys. Lett.* A **77** 153–5
Bely O 1966 *Proc. Phys. Soc.* **87** 1010–1
—— 1967 *Nuovo Cim.* **49** 66–86
Bhatia A K and Temkin A 1977 *J. Phys. B: At. Mol. Phys.* **10** 2893–912
Burgess A, Hummer D G and Tully J A 1970 *Phil. Trans. R. Soc.* A **266** 225–79
Das A K, Maiti N and Sil N C 1978 *Indian J. Phys.* B **52** 83–97
Henry R J W 1981 *Phys. Rep.* **68** 3–91
McDowell M R C, Morgan L A, Myerscough V P and Scott T 1977 *J. Phys. B: At. Mol. Phys.* **10** 2727–38
Magee N H, Mann J B, Merts A L and Robb W D 1977 *Los Alamos Scientific Laboratory Report* LA-6691-MS
Morse P M, Young L A and Haurwitz E S 1935 *Phys. Rev.* **48** 948–54
Nakazaki S 1978 *J. Phys. Soc. Japan* **45** 225–9
Ochkur V I 1964 *Sov. Phys.–JETP* **18** 503–8
Rudge M R H 1965 *Proc. Phys. Soc.* **85** 607–8
—— 1965 *Proc. Phys. Soc.* **86** 763–72
Seaton M J 1975 *Advances in Atomic and Molecular Physics* vol 11, ed D R Bates and B Bederson (New York: Academic) pp 83–142
Tully J A 1980 *J. Phys. B: At. Mol. Phys.* **13** 3023–34
Wyngaarden W L, Bhadra K and Henry R J W 1979 *Phys. Rev.* A **20** 1409–17