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Theoretical calculation of electron-impact resonance excitation of alkali atoms

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Abstract. Total cross-section for electron impact excitation of the resonance levels in Li, Na and K are calculated using the method due to Crothers and McCarroll. The results are compared with other available theoretical and experimental data.

Keywords. Electron-impact excitation; resonance transitions; alkali atoms.

In a previous paper, Srivastava and Rai (1978) studied the electron impact excitation of hydrogen and helium using the method suggested by Crothers and McCarroll (1965) which will be referred hereafter as MCM. The reasonable success of such a study encouraged us to extend these calculations to excitation of the alkali atoms. In particular, the resonance excitation of the type $ns^2S \rightarrow np^2P$ in alkali metal atoms (due to electron impact) is known to have a very large cross-section which makes this transition suitable for study by two -state (coupling) treatment like MCM.

Several theoretical and experimental results are already available in literature (see for example a recent paper of Kennedy *et al* 1977) on the electron-impact resonance excitation of alkali atoms but many discrepancies and ambiguities remain. In order to have a meaningful comparison among different theories, it is desirable to compare the results obtained using identical wavefunctions. We felt, therefore, that if the same wavefunctions as used in other studies (Walters 1973; Kennedy *et al* 1977) are used in MCM, one can test the suitability of the MCM method for this purpose. It may be noted that Crothers and McCarroll (1965) in their original work had also reported results for the $3s \rightarrow 3p$ excitation in sodium but had used different wavefunctions.

In the present note, we report our calculated total cross-sections using MCM for the following resonance transitions:

$$e^- + \mathrm{Li}(2s) \rightarrow e^- + \mathrm{Li}(2p)$$

$$e^- + \mathrm{Na}(3s) \rightarrow e^- + \mathrm{Na}(3p)$$

$$e^- + \mathrm{K}(4s) \rightarrow e^- + \mathrm{K}(4p)$$

The details of the theoretical model and the numerical evaluation of the cross-section have been reported earlier (Srivastava and Rai 1978). The effect of electron ex-

change has now been studied by following an approach similar to the Ochkur approximation.

The ground state of lithium has been represented by the wavefunction due to Clementi (1965) while the function for the $2p$ orbital has been taken from Vinkalns *et al* (1964). The wavefunctions of Szasz and McGinn (1967) have been used for the np orbitals of sodium ($n=3$) and potassium ($n=4$). In these later calculations the core orbitals (for example $1s$, $2s$ and $2p$ in the case of Na) are mutually orthogonal but the valence orbitals ($3s$ and $3p$ in Na) are not orthogonal to the core orbitals and reorthogonalization is needed. The final orbitals after reorthonormalization are of the form

$$\Psi_{3p}(r) = a_1 \Phi_{3p}(r) + a_2 \Phi_{2p}(r)$$

$$\Psi_{3s}(r) = a_1' \Phi_{3s}(r) + a_2' \Phi_{2s}(r) + a_3' \Phi_{1s}(r) \qquad \text{(for Na)}$$

and

$$\Psi_{4p}(r) = b_1 \Phi_{4p}(r) + b_2 \Phi_{3p}(r) + b_3 \Phi_{2p}(r)$$

$$\Psi_{4s}(r) = b_1' \Phi_{4s}(r) + b_2' \Phi_{3s}(r) + b_3' \Phi_{2s}(r) + b_4' \Phi_{1s}(r) \qquad \text{(for K)}$$

Table 1. Total cross-sections (in πa_0^2)

Impact Energy (eV)	Li		Na		K	
	With Exchange	Without Exchange	With Exchange	Without Exchange	With Exchange	Without Exchange
5	3·27(1)*	2·54(1)	1·97(1)	1·79(1)	3·33(1)	3·27(1)
7	2·52(1)	2·38(1)	2·01(1)	1·96(1)	3.83(1)	3·79(1)
9	2·48(1)	2·43(1)	2·22(1)	2·19(1)	4·22(1)	4·19(1)
10	2·50(1)	2·46(1)	2·31(1)	2·28(1)	4·36(1)	4·33(1)
11	—	—	2·38(1)	2·36(1)	4·48(1)	4·45(1)
13	—	—	2·50(1)	2·47(1)	4·63(1)	4·60(1)
15	—	—	2·57(1)	2·55(1)	4·70(1)	4·68(1)
17	—	—	2·61(1)	2·59(1)	4·73(1)	4·70(1)
19	—	—	2·63(1)	2·61(1)	4·71(1)	4·69(1)
20	2·52(1)	2·50(1)	2·63(1)	2·61(1)	4·70(1)	4·69(1)
30	2·33(1)	2·32(1)	2·51(1)	2·50(1)	4·36(1)	4·35(1)
40	2·12(1)	2·11(1)	2·32(1)	2·31(1)	3·96(1)	3·95(1)
50	1·93(1)	1·93(1)	2·13(1)	2·12(1)	3·60(1)	3·60(1)
60	1·77(1)	1·76(1)	1·96(1)	1·96(1)	3·29(1)	3·29(1)
62	1·74(1)	1·74(1)	1·93(1)	1·93(1)	3·24(1)	3·23(1)
64	1·71(1)	1·71(1)	1·90(1)	1·90(1)	3·18(1)	3·18(1)
66	1·68(1)	1·68(1)	1·87(1)	1·87(1)	3·13(1)	3·13(1)
70	1·63(1)	1·63(1)	1·81(1)	1·81(1)	3·03(1)	3·03(1)
80	1·51(1)	1·51(1)	1·69(1)	1·68(1)	2·80(1)	2·80(1)
100	1·32(1)	1·32(1)	1·48(1)	1·48(1)	2·44(1)	2·44(1)
120	1·17(1)	1·17(1)	1·32(1)	1·32(1)	2·17(1)	2·17(1)
150	1·01(1)	1·01(1)	1·13(1)	1·13(1)	1·86(1)	1·86(1)
170	9·22	9·22	1·04(1)	1·04(1)	1·70(1)	1·70(1)
200	8·19	8·19	9·24	9·24	1·51(1)	1·51(1)
250	6·92	6·93	7·83	7·83	1·27(1)	1·27(1)
300	6·01	6·01	6·80	6·81	1·10(1)	1·10(1)
400	4·78	4·78	5·42	5·42	8·72	8·72
500	3·97	3·98	4·52	4·52	7·23	7·23

*The integers in brackets indicate the power of ten by which the corresponding number is to be multiplied.

The different $\Phi(r)$ functions are taken from Szasz and McGinn (1967). The calculation of the values of $a_i s$, $a_i' s$, $b_i s$ and $b_i' s$ (given below) is straightforward but lengthy,

$$a_1 = 1{\cdot}00621 \text{ and } a_2 = -0{\cdot}111661;$$

$$a_1' = 1{\cdot}02521,\ a_2' = 0{\cdot}22488 \text{ and } a_3' = -0{\cdot}02195$$

$$b_1 = 1{\cdot}01704,\ b_2 = -0{\cdot}18474 \text{ and } b_3 = -0{\cdot}01548$$

$$b_1 = 1{\cdot}05076,\ b_2' = -0{\cdot}31751,\ b_3' = -0{\cdot}05712 \text{ and } b_4' = -0{\cdot}00548$$

Our calculated cross-section results are shown in table 1 and are also displayed in figures 1 to 3 along with other theoretical and experimental results.

In figure 1, we compare the experimental results of Leep and Gallagher (1974) and Williams *et al* (1976) for the total $2s \rightarrow 2p$ excitation cross-section of lithium with our results as well as of the unitarised distorted wave-polarized orbital model (UDWPO II)

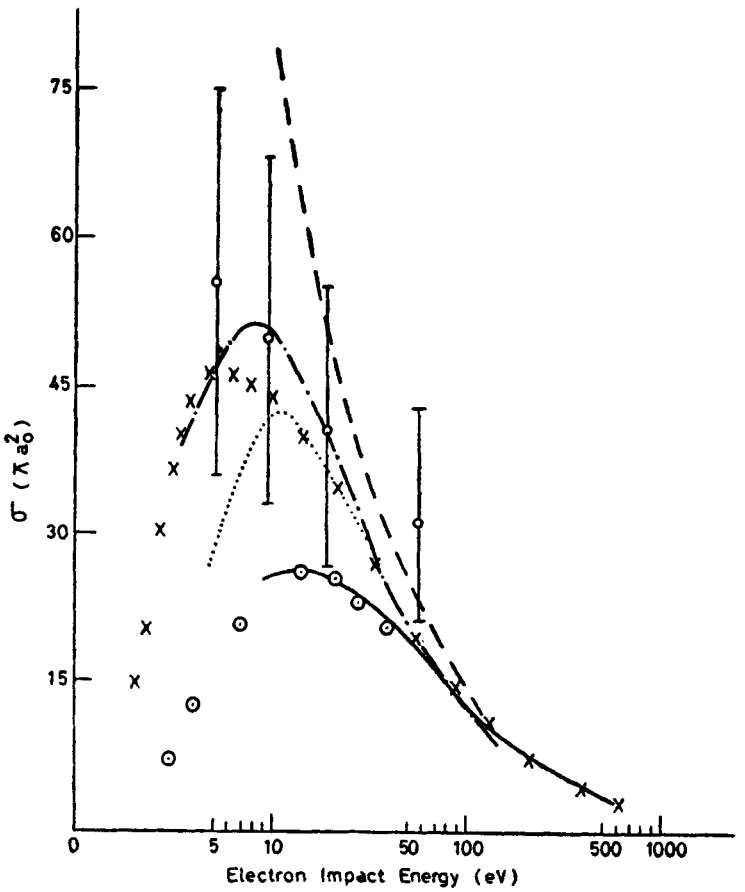

Figure 1. Total cross section for the resonance transition of Li. Experimental results: ◊ Williams *et al* (1976) and x Leep and Gallagher (1974).
Theoretical results: — Present; — · — UDWPO II - - - - FBA; ..... GA. ○ FF.

(Kennedy *et al* 1977), first Born approximation (FBA) (Walters 1973) and Glauber approximation (GA) (Walters 1973). The present results agree with experiments and other theories for electron impact energies greater than 50 eV. For energies below 50 eV the cross-section is underestimated by the MCM but in view of the large uncertainties (obvious from the error bars) attached to the more recent experimental data of Williams *et al* (1976), these can still be regarded as reasonable up to as low an impact energy as 20 eV. Values due to Felden and Felden (1973) FF who use a semi-empirical correlation model are also shown.

Figure 2 shows the results for $3s \rightarrow 3p$ resonance excitation in Na. We display and compare our results with the same set UDWPO II, FBA, GA and FF of theoretical results as mentioned earlier. The experimental results are due to Enemark and Gallagher (1972). We observe that the agreement of our results with experiment is better than for lithium. The overall agreement is also much better than other theoretical results. It can also be concluded that at low impact energies (< 50 eV), the present MCM results underestimate the cross-section while UDWPO II model overestimates it.

Finally, our total cross-section results for $4s \rightarrow 4p$ excitation in potassium are compared in figure 3 where in addition to the FBA, GA, FF and UDWPO II calculations the two sets of recent experimental data are also shown (Zapesochnyi *et al* 1975 and Williams and Trajmar 1977). In this case the experimental results due to Williams and Trajmar (1977) at low and intermediate energies show large deviations from the results of Zapesochnyi *et al* (1975). This is surprising since the results from lithium showed close agreement (Kennedy *et al* 1977).We find that the present MCM results are in better agreement with the experimental results of Williams and Trajmar (1977).

From the present results as well as those of Kennedy *et al* (1977) it is clear that further experimental and theoretical studies are necessary. Further, MCM can be

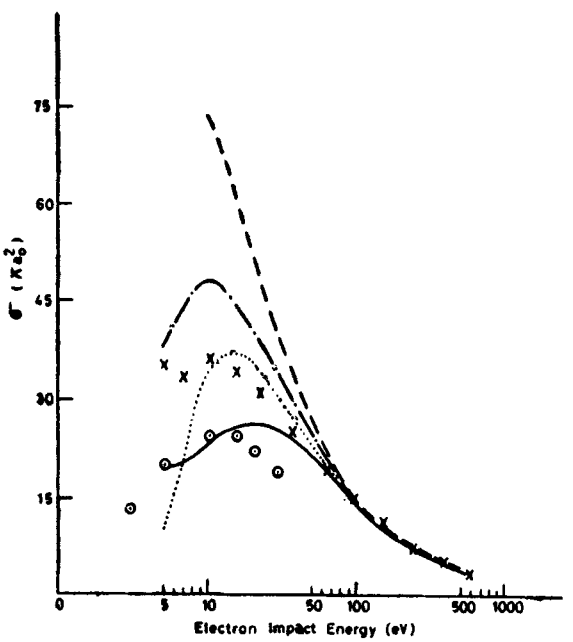

Figure 2. Total cross-section for the resonance transition of Na. Experimental results: x Enemark and Gallagher (1972). Theoretical results: Same as in figure 1.

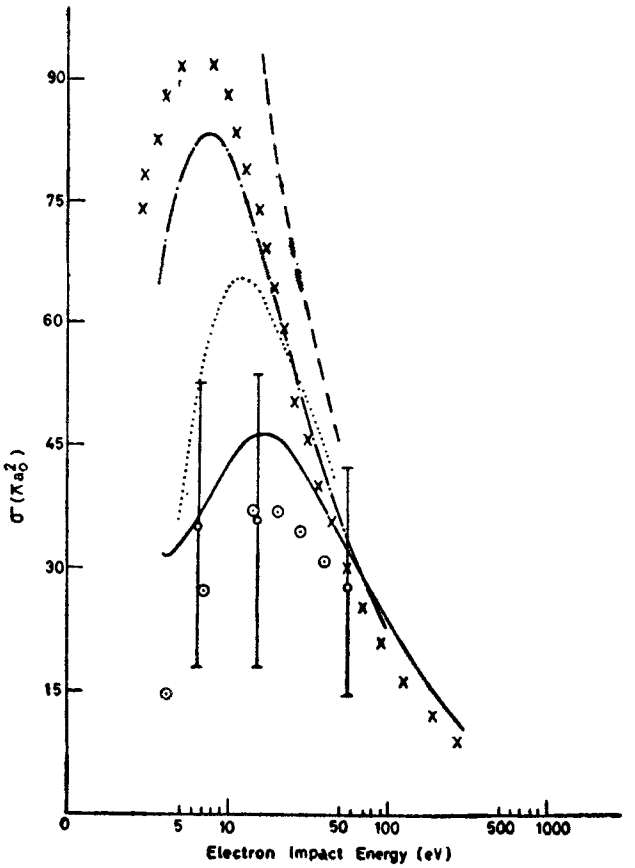

Figure 3. Total cross-section for the resonance transition of K. Experimental results: x Zapesochnyi *et al* (1975) ♀ Williams and Trajmar (1977). Theoretical results: same as in figure 1.

treated as a reasonably good and economical approximation at least for intermediate and high impact energies. The success of MCM has also been recently demonstrated by Srivastava *et al* (1982) in their study of excitation of the autoionizing levels in alkalis. To estimate the contribution due to exchange effects and to compare their effect with the MCM results, we have applied an Ochkur type correction for exchange effects in all cases. It is found that the exchange contribution above 50 eV is small and at low impact energies this increases the MCM cross-sections. It is obvious that this approximate correction improves the overall agreement of our calculated results with experimental values. We feel that with proper evaluation of exchange effects MCM would become a still more accurate description.

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References

Clementi E 1965 *Tables of Atomic Functions* (San Jose: IBM)
Crother D S F and McCarroll R 1965 *Proc. Phys. Soc.* **86** 753
Enemark E A and Gallagher A 1972 *Phys. Rev.* **A6** 192
Felden M M and Felden M A 1973 *Can. J. Phys.* **51** 1709
Kennedy J V, Myerscough V P and McDowell M R C 1977 *J. Phys.* **B10** 3759
Leep D and Gallagher A 1974 *Phys. Rev.* **A10** 1082
Srivastava R and Rai D K 1978 *J. Phys.* **B11** 309
Srivastava R, Singh C S and Rai D K 1982 *J. Phys.* **B15** 1899
Szasz L and McGinn G 1967 *J. Chem. Phys.* **47** 3495
Vinkalns Zh., Karule E M and Obedkov V D 1964 *Opt. Spectrosc.* **17** 105
Walters H R J 1973 *J. Phys.* **B6** 1003
Williams W, Trajmar S and Bonzinis 1976 *J. Phys.* **B9** 1529
Williams W and Trajmar S 1977 *J. Phys.* **B10** 1955
Zapasochnyi I P, Postoi E N and Alekshakhin I S 1975 *Sov. Phys. JETP* **41** 865