J. Phys. B: Atom. Molec. Phys., Vol. 10, No. 18, 1977. Printed in Great Britain.

Electron impact excitation of the resonance transitions of Li, Na and K

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Received 3 June 1977, in final form 23 August 1977

Abstract. A unitarised distorted-wave polarised-orbital model is used to investigate electron impact excitation of the Li, Na and K resonance transitions at low and intermediate energies. Results are presented for integral (total) cross sections, differential cross sections, coincidence parameters, and, for K, spin-flip differential cross sections. They are compared where possible with experiment and other theoretical models. The evaluation of the adiabatic polarisation interaction is discussed. Core-exchange effects are investigated for the case of Na. Tables of T-matrix elements are available for all three cases to aid in interpretation of photon–electron coincidence experiments.

1. Introduction

We report theoretical results in a distorted-wave approximation for the resonance transitions of the light alkali metals, namely Li, Na and K; the model used is an extension of the distorted-wave polarised-orbital model (DWPO) of McDowell *et al* (1973, 1974, 1975). The resonance transition of the type $ns\,^2S \rightarrow np\,^2P$ is strong, with a very large cross section, and is particularly suited to a two-state treatment since coupling to other states is relatively unimportant. There has been extensive earlier theoretical work ranging from the first Born approximation (FBA) to many-state close-coupling treatments. The published close-coupling treatments, except for Burke and Taylors' (1969) two-state calculations for Li, have been restricted to very low energies, or have neglected exchange. Further, most of the work has been restricted to total cross sections and small-angle differential cross sections. Rather than list all the theoretical papers in this introduction, we refer to them below when making comparison of our results with them and, where possible, with experiment. A full review is in course of publication (Bransden and McDowell 1977, 1978).

The experimental work available for comparison is extensive, though most of it is normalised (i.e. relative rather than absolute measurements) and includes integrated cross sections and polarisation fractions by a JILA group (Li: Leep and Gallagher 1974; Na: Enemark and Gallagher 1972) and integrated and differential cross sections by Trajmar and his colleagues (Li: Williams *et al* 1976; K: Williams and Trajmar 1977) as well as earlier work quoted in these references. Important

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measurements of the optical excitation function have been reported by Zapesochnyi's group (Zapesochnyi 1967) and more recently by Zapesochnyi *et al* (1975). There are recent differential measurements for Na by Shuttleworth *et al* (1977) and a time-reversed photon–electron coincidence experiment for the Na resonance transition by Hertel and Reiland (Reiland 1976; see also Hermann *et al* 1977). All of these will be discussed in §3. However, we first present a brief review of our theoretical model in §2 stressing only those points where it departs from our earlier work.

2. Theory

A full account of the theoretical model is given elsewhere (Kennedy 1976). The model is based on evaluating an approximation to the exact singlet and triplet T-matrix elements, $T_{if}^{\pm}$. This approximation includes exchange and the effects of adiabatic dipole distortion of the initial state by the incident electron, but replaces the unknown total scattering function Ψ_i^+ by the adiabatic exchange approximation to its elastic scattering part (Drachman and Temkin 1972). Exchange polarisation is neglected, but core-distortion effects are examined in some detail for Na. Finally the cross sections obtained are unitarised in the manner suggested by Seaton (1961). Unitarisation reduces our values by up to 40% near threshold, but rapidly becomes less important with increasing energy. The effect is comparable with that which we obtain in Born and Born–Oppenheimer calculations (Kennedy 1976). We note that this method has given accurate results for transitions from the ground state to excited s and p states (of the same symmetry) in H and He (cf McDowell *et al* 1975, Scott and McDowell 1976) at energies above the first ionisation threshold. Non-adiabatic terms could be significant at high energies (cf Walters 1976, for a discussion of these effects in elastic scattering). We thus present our results only up to energies of about fifty times threshold. At higher energies, the FBA should be adequate for total cross sections.

In calculating approximations to the T-matrix elements

$$T_{if} = \langle \phi_f | V | \Psi_i^+ \rangle$$

the approximation made for Ψ_i^+ need not be accurate asymptotically, provided

(i) the electron density is small in the asymptotic region,

(ii) exchange contributions are small compared with direct (cf Byron and Joachain 1977, who use this argument to justify an elastic channel eikonal approximation to Ψ_i^+).

2.1. The polarisation potential

The unperturbed atomic orbitals were approximated for Li by the wavefunctions of Clementi (1965) with the 2p valence orbital taken from Gailitis (see Vinkalns *et al* 1964). The wavefunctions of Szasz and McGinn (1967) were adopted for Na and K and, following Walters (1973), the valence orbitals were explicitly orthogonalised to the core functions.

In order to obtain the adiabatic exchange elastic-scattering distorted wave and the adiabatic dipole distorted initial state, we must first obtain the adiabatic dipole polarisation potential. Following Stone (1966), we write the adiabatic distorted initial

state for the valence ns electron (with position vector r_2) perturbed by the incident electron (with position vector r_1) as

$$\psi(2) = \phi_{ns}(2) + \phi_{pol}(1, 2) \tag{1}$$

where

$$\phi_{pol}(1, 2) = \beta(r_1)\phi_{np}(2) \tag{2}$$

and ϕ_{ns}, ϕ_{np} are the ground- and first-excited-state functions. $\beta(r_1)$ is then determined by variational minimisation of the perturbed ground-state energy, which, together with the requirement that β be everywhere negative (to ensure an attractive potential), leads to

$$\beta(r_1) = -\left|\left|\frac{T}{K}\right| - \left(\frac{T^2}{K^2} + 4\right)^{1/2}\right| \tag{3}$$

(cf Vo Ky Lan 1972). Here

$$\begin{aligned} K &= V_{ns,np} \\ T &= \epsilon_{np} - \epsilon_{ns} + V_{np,np} - V_{ns,ns} \end{aligned} \tag{4}$$

with the energies in rydbergs and the interaction matrix elements $V_{nl,nl'}$ given by

$$V_{nl,nl'} = \langle \phi_{nl} | V | \phi_{nl'} \rangle \tag{5}$$

with

$$V = \frac{2}{r_{12}} - \frac{2}{r_1} \qquad \text{Ryd} \tag{6}$$

assuming a fixed core. The polarisation potential is then given by

$$V_{pol}(r_1) = \beta(r_1)V_{ns,np} \qquad \text{Ryd.} \tag{7}$$

The results obtained for Na using equation (7) for V_{pol} agree well with those of Vo Ky Lan (1971) using the Sternheimer approximation and with those from a Callaway–Temkin hydrogenic potential (see e.g. Drachman and Temkin 1972) scaled to the experimental polarisability of Na.

As a further test of our polarisation potential, we solved the exchange adiabatic equations for elastic scattering of electrons by Na, from threshold to 2 eV, with and without exchange with the core, and compared our results for the elastic-scattering phaseshift with those of the two-state close-coupling calculations (Norcross 1971); we note that the above two-state results agree well with the four-state calculations of Moores and Norcross (1972). The agreement between our results and Norcross (1971) is satisfactory for ^{1}S, ^{3}S and ^{1}P, but poor for ^{3}P where (as expected) we fail to obtain a resonance in this model. In fact, this is of no consequence in our main calculations since we are interested in energies above the inelastic threshold, and, moreover, it has been demonstrated (by Vo Ky Lan 1971) that inclusion of exchange polarisation produces a ^{3}P phaseshift in good agreement with the close-coupling results.

2.2. Evaluation of the T matrix and the observables

Having solved the adiabatic exchange equation using $V_{\rm pol}(r_1)$ of equation (7), the problem then reduces to that of the two-electron systems, for which the full analysis has been given by Syms *et al* (1975), provided that we

(i) replace $\beta(r_1)$ by $\epsilon(r_1, r_2)\beta(r_1)$ (Drachman and Temkin 1972) in evaluating the matrix elements, where

$$\epsilon(r_1, r_2) = \begin{cases} 1 & r_2 < r_1 \\ 0 & \text{otherwise,} \end{cases} \tag{8}$$

(ii) neglect core-exchange terms in the matrix elements.

With these approximations there is therefore no need to repeat the analysis. The inclusion of core exchange is discussed in detail by Kennedy (1976); the analysis is lengthy but straightforward and need not be reproduced here. Results obtained for the Na resonance transition are reported in §3.

2.3. Unitarisation

The singlet and triplet T matrices, $\mathbf{T}^{\pm}$, are related to the S matrices by

$$\mathbf{S}^{\pm} = \mathbf{I} - \mathbf{T}^{\pm} \tag{9}$$

where $\mathbf{I}$ is the unit matrix. We wish to ensure unitarity of $\mathbf{S}^{\pm}$. Introducing the real symmetric $\mathbf{R}$ matrix through

$$\mathbf{T}^{\pm} = -2\mathrm{i}\mathbf{R}^{\pm}(\mathbf{I} - \mathrm{i}\mathbf{R}^{\pm})^{-1} \tag{10}$$

a first approximation is

$$\mathbf{T}^{\pm} = -2\mathrm{i}\mathbf{R}^{\pm} \tag{11}$$

provided that, for a given transition $\Gamma \rightarrow \Gamma'$ (in the coupled $LS\pi$ representation) each element of the R matrix satisfies

$$|R^{\pm}_{\Gamma\Gamma'}| \ll 1 \tag{12}$$

(Seaton 1961). If (12) holds, the appropriate elements of $\mathbf{S}$ are constructed from (11), otherwise (11) is used to obtain a first estimate, $\mathbf{R}^{\pm}(0)$, which is inserted in (10) to ensure that $\mathbf{S}$ is unitarised.

In our case, however, due to the explicit phase factors, we are not using a purely imaginary T matrix as in the FBA, and thus we cannot adopt this approach with a real symmetric matrix $\mathbf{R}^{\pm}$. Instead, after transferring to the coupled representation (Γ), we construct a matrix $\mathbf{K}^{\pm}$ with the elements $T^{\pm}_{\Gamma\Gamma'}(0)$ as the upper triangle and the lower triangular elements chosen so that $\mathbf{K}^{\pm}$ is Hermitian. Then a second approximation to the T matrix (which ensures unitarity of the S matrix) is

$$\mathbf{T}^{\pm}(1) = -2\mathrm{i}\mathbf{K}^{\pm}(\mathbf{I} - \mathrm{i}\mathbf{K}^{\pm})^{-1}. \tag{13}$$

Consider, for example, an ns–np transition in which it is assumed that the only non-vanishing elements of $\mathbf{T}^{\pm}(0)$ are

$$\begin{aligned} T^{\pm}(ns, np, L, L-1) &= -2\mathrm{i}\exp(\mathrm{i}\Delta^{\pm}_{L,L-1})\alpha^{\pm} \\ T^{\pm}(ns, np, L, L+1) &= -2\mathrm{i}\exp(\mathrm{i}\Delta^{\pm}_{L,L+1})\beta^{\pm} \end{aligned} \tag{14}$$

where $\alpha^{\pm}$, $\beta^{\pm}$ are real and $\Delta^{\pm}_{L,L\pm1}$ are the appropriate phase factors. Then, omitting the superscripts $\pm$ for clarity, $\mathbf{K}$ takes the form

$$\mathbf{K} = \begin{bmatrix} 0 & \exp(i\Delta_{L,L-1})\alpha & \exp(i\Delta_{L,L+1})\beta \\ \exp(-i\Delta_{L,L-1})\alpha & 0 & 0 \\ \exp(-i\Delta_{L,L+1})\beta & 0 & 0 \end{bmatrix} \tag{15}$$

which leads to

$$\mathbf{T}(1) = -\frac{2i}{1+\alpha^2+\beta^2}\begin{bmatrix} i(\alpha^2+\beta^2) & \alpha\exp(i\Delta_{L,L-1}) & \beta\exp(i\Delta_{L,L+1}) \\ \alpha\exp(-i\Delta_{L,L-1}) & i\alpha^2 & i\alpha\beta\exp[i(\Delta_{L,L+1}-\Delta_{L,L-1})] \\ \beta\exp(-i\Delta_{L,L+1}) & i\alpha\beta\exp[i(\Delta_{L,L-1}-\Delta_{L,L+1})] & i\beta^2 \end{bmatrix} \tag{16}$$

and $\mathbf{S}$ is unitary.

We adopted this procedure and, having calculated $\mathbf{T}^{\pm}(1)$ in the coupled representation, transformed back to the uncoupled representation in terms of the orbital angular momenta of the individual states to evaluate cross sections for excitation of specific magnetic sub-levels. The partial-wave T-matrix elements were then summed over L to give the singlet and triplet T matrices for excitation to the $|np\,M_L\rangle$ state, $T^{\pm}(M_L)$, which are complex quantities.

2.4. Contributions from large angular momentum

For s–p transitions the electron–atom interaction is long range, and many angular momenta contribute. This raises particular difficulty in obtaining accurate large-angle differential cross sections. For example, we find that for satisfactory convergence of the inelastic differential cross section at $k^2 = 1$ Ryd, at $\theta > 120°$, more than 150 partial waves need to be included.

We therefore adopt the procedure of McDowell *et al* (1975) and subtract the non-unitarised Born, polarised Born, or Born exchange partial-wave T-matrix elements from the corresponding direct, polarised direct, and exchange unitarised DWPO matrix elements for all $L \leqslant L_0$, where L_0 is sufficiently large that unitarisation is no longer important. We then add the full Born, polarised Born or Born exchange matrix elements to these matrix elements. We find that L_0 varies between 20 and 50, depending on the element and energy considered; we tested our results for insensitivity to the choice of L_0. Details of the analysis are given by Kennedy (1976).

3. Results

3.1. Lithium

3.1.1. Integral cross sections. Our results for the integrated (total) cross sections for the transition

$$e^- + Li(2^2S) \rightarrow e^- + Li(2^2P)$$

are given in table 1, in both the DWPO I model (neglecting target distortion) and in the full DWPO II model. In each case the non-unitarised results are denoted by Q I, the unitarised by Q II. The results are presented at selected energies, the lowest

Table 1. Integral (total) cross sections (πa_0^2) for $e^- + Li(2^2S) \rightarrow e^- + Li(2^2P)$.

	DWPO I		DWPO II	
E(eV)	Q I	Q II	Q I	Q II
5·1	95·1	57·3	72·6	46·9
8·1	86·8	67·3	67·2	51·4
12·1	72·5	58·3	57·4	48·7
27·2	43·9	39·9	36·2	33·9
54·4	26·1	25·0	22·3	21·6
100·0	—	—	13·9	13·7
200·0	—	—	8·01	7·97

Q I refers to the non-unitarised, Q II to the unitarised result, in each case.

three of these being chosen to match those used by Hertel in his coincidence experiments on Na (see §3.2). Target distortion appreciably reduces the cross section at low energies, and unitarisation has an even stronger effect, particularly in the DWPO I model. Comparison with other theoretical models and with experiment is made in figures 1 and 2. Accurate FBA values have been calculated by many workers including ourselves (see Bell and Kingston 1974); we illustrate those of Walters (1973), with which we agree, as we used the same wavefunctions. A restricted eikonal (Glauber) model has also been presented by Walters (1973) while two-state close-coupling calculations have been reported by Burke and Taylor (1969) at energies up to 54·4 eV, and by Issa (1977), his results being larger than those of Burke and Taylor by between 5 and 8%. (This difference is probably due to the choice of approximate target wavefunctions; a fuller discussion is given elsewhere (Bransden and McDowell 1978).)

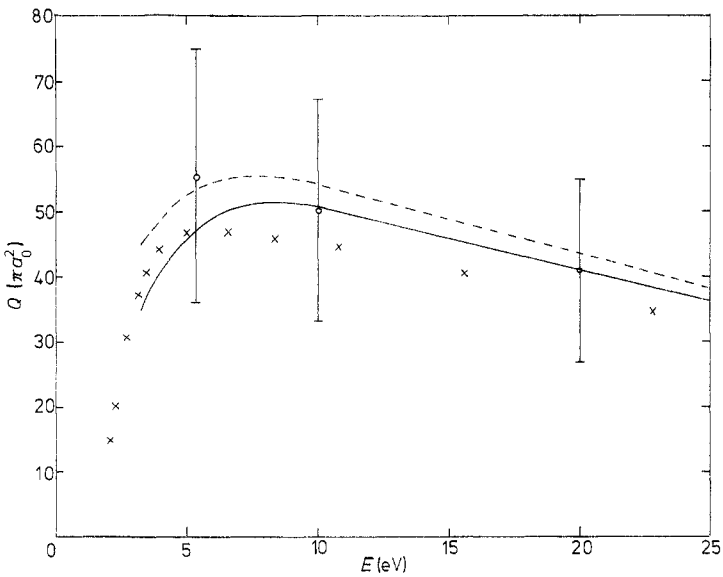

Figure 1. Integrated (total) cross sections (πa_0^2) for the resonance transition of Li from 0 to 25 eV. Experimental results: ○ Williams *et al* (1976); × Leep and Gallagher (1974). Theoretical results: – – – – two-state close-coupling (Burke and Taylor 1969); —— UDWPO II (this paper).

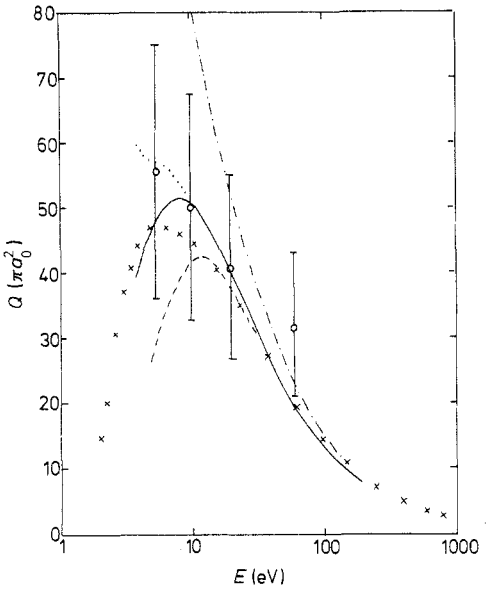

Figure 2. Integrated (total) cross sections (πa_0^2) for the resonance transition of Li to 1 keV. Experimental results: ⊖ Williams *et al* (1976); × Leep and Gallagher (1974). Theoretical results: –·–·– FBA (Walters 1973); – – – – Glauber (Walters 1973); ····· McCavert and Rudge (1972); —— UDWPO II (this paper).

The experimental measurements of Hughes and Hendrickson (1964), normalised to an early value by Haft (1933) in Na, are in good agreement with the relative measurements of Leep and Gallagher (1974), normalised to the FBA at 1·404 keV and corrected for polarisation and cascade effects. (The latter authors do not list their anticipated uncertainties for the excitation cross section.) The optical excitation results of Aleksakhin and Zapesochnyi (1967) lead to absolute values of the excitation cross section about a factor of two lower at low and intermediate energies than those of Hughes and Hendrickson or Leep and Gallagher. It was suggested by Leep and Gallagher that this might be due partly to the effect of resonance trapping in the atomic beam used by Aleksakhin and Zapesochnyi. More recent optical excitation work by Zapesochnyi *et al* (1975) includes this effect and gives values for the excitation cross section which agree almost identically with the results obtained by Williams *et al* (1976) over the range 5–20 eV. Williams *et al* measured differential cross sections, integrated these results, and normalised the sum of the elastic plus inelastic integral cross sections to the difference between the total cross sections of Kasdan *et al* (1971) and the ionisation cross section. Williams *et al* estimate the uncertainties involved in this procedure for the excitation cross section to be $\pm 35\%$, but their results are consistent with the data of Leep and Gallagher over the energy range considered, with the exception of the point at 60 eV which lies 40% higher than that of Zapesochnyi *et al* and about 60% higher than that of Leep and Gallagher. From an analysis of the total elastic, inelastic and ionisation cross sections, Walters (1976) suggests that the experimental data of Kasdan *et al* (1971) for the total cross section of lithium may be too high and should possibly be renormalised by a factor of 0·76; there may also be an energy-dependent error in the measurements leading to cross sections which are too large at energies greater than about 50 eV.

In figure 1 we compare the experimental results of Leep and Gallagher and Williams *et al*, for the integrated 2s–2p excitation cross section of lithium from threshold to 20 eV, with our UDWPO II calculations and the two-state close-coupling values of Burke and Taylor (1969). Clearly, both the theoretical models are in good agreement with the experiments. Results over a wider range of energies are shown in figure 2; we give the FBA and Glauber (Walters 1973), McCavert–Rudge model (McCavert and Rudge 1972) and the UDWPO II theoretical results, and compare these with the experimental data discussed above. The FBA fails, as expected, at low energies, but in view of the large uncertainties attached to the experimental data of Williams *et al*, may be consistent with experiment to energies as low as ten times threshold. The Glauber model agrees well to slightly lower energies before beginning to underestimate the cross section, but its success is very probably fortuitous; a detailed criticism is given elsewhere (Bransden and McDowell 1977). The McCavert–Rudge model gives results which are in close agreement with the data of Williams *et al* over the range 4–10 eV (see, however, §§3.2 and 3.3). It is of interest to note that the two-state close-coupling (with second-order potential) calculations of Issa (1977) (see Bransden and McDowell 1978) are in close accord with the present UDWPO II results. However, the values of Felden and Felden (1973) in a semi-empirical correlation model are approximately a factor of two lower at energies below 30 eV.

From figures 1 and 2 we see that the UDWPO II results for the resonance transition in lithium are consistent with the close-coupling calculations and with the experimental data at all available energies. As pointed out for the (1^1S–n^1S) and (1^1S–n^1P) transitions in helium (Scott and McDowell 1975, 1976) this is because the UDWPO II model accurately describes the forward cross sections above the first ionisation threshold.

3.1.2. Differential cross sections. Calculated differential cross sections in the UDWPO II model are given in table 2 at selected energies and angles. The results at 20 eV are compared with the experimental measurements of Williams *et al* (1976) in figure 3. The agreement is reasonably good out to 70°, the failure of the theory at large angles being expected, and due, among other effects, to neglect of final channel distortion (Bransden and McDowell 1977). It strongly supports the normalisation adopted

Table 2. UDWPO II inelastic differential cross sections ($a_0^2\,sr^{-1}$) for the resonance transition of Li.

θ(deg) \ E(eV)	5·1	12·1	20·0	27·2	54·4	100
0	6·97 + 02	3·29 + 03	6·29 + 03	9·02 + 03	1·91 + 04	3·59 + 04
5	5·73 + 02	1·36 + 03	1·21 + 03	9·68 + 02	4·62 + 02	2·03 + 02
10	3·50 + 02	3·79 + 02	2·31 + 02	1·56 + 02	5·46 + 01	1·78 + 01
15	1·85 + 02	1·20 + 02	6·20 + 01	3·85 + 01	1·08 + 01	2·63 + 00
20	9·19 + 01	4·33 + 01	2·04 + 01	1·20 + 01	2·72 + 00	4·77 − 01
25	4·48 + 01	1·74 + 01	7·75 + 00	4·30 + 00	8·09 − 01	1·52 − 01
30	2·21 + 01	7·72 + 00	3·31 + 00	1·75 + 00	3·25 − 01	7·04 − 02
60	3·17 + 00	4·61 − 01	1·90 − 01	1·19 − 01	3·72 − 02	1·13 − 02
90	1·54 + 00	1·68 − 01	9·82 − 02	6·60 − 02	1·90 − 02	5·33 − 03
120	7·52 − 01	1·90 − 01	9·70 − 02	5·81 − 02	1·45 − 02	3·60 − 03
150	3·42 − 01	2·22 − 01	9·86 − 02	5·61 − 02	1·31 − 02	3·12 − 03
180	5·71 − 02	2·26 − 01	9·61 − 02	5·08 − 02	1·03 − 02	2·36 − 03

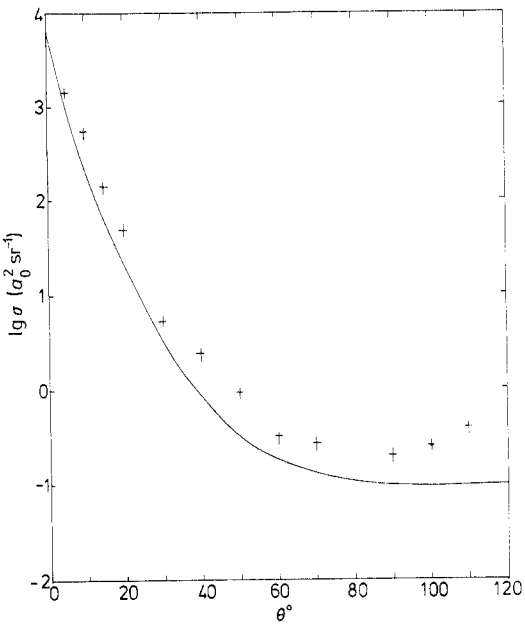

Figure 3. Differential cross sections ($a_0^2\,\mathrm{sr}^{-1}$) for the resonance transition in Li at 20 eV. Experimental results: + Williams *et al* (1976); the anticipated uncertainties are ±35%. Theoretical results: —— UDWPO II (this paper).

by Williams *et al* (1976) and suggests that, at least near 20 eV, their adopted integral cross section (41 πa_0^2 at this energy) has an error of much less than the quoted ±35%.

3.1.3. Orientation and alignment parameters. Although no electron–photon coincidence experiments, or time-reversed such experiments, have yet been reported for the $2^2S \rightarrow 2^2P$ transition of Li, work is in progress at several laboratories. Such measurements are equivalent to measurements of the linear and circular polarisation of the emitted light, and the results can be expressed in the form of Stokes parameters, or equivalently Fano–Macek parameters (Kleinpoppen 1976). The theory for the alkalis is identical to that for hydrogen (neglecting fine-structure splitting) given by Morgan and McDowell (1975) and need not be repeated here. For the convenience of experimentalists we have available tables of the real and imaginary parts of the T matrices, $T^{\pm}(M_L)$, summed over all partial waves, for both singlet and triplet contributions to both $M_L = 0$ and $M_L = \pm 1$ transitions. Using the above references, these may easily be expressed in whatever form the experimental physicist requires. As an example, the λ parameter

$$\lambda = \frac{\sigma(M_L = 0)}{\sigma(M_L = 0) + 2\sigma(M_L = 1)}$$

where $\sigma(M_L)$ is the differential cross section for excitation of the $2^2P(M_L)$ magnetic sub-level, is shown in figure 4. The behaviour is similar to that previously reported by several groups for $H(2^2P)$. In view of our agreement with Williams *et al*'s measurements of the total differential cross section, we would expect λ values deduced from $T^{\pm}(M_L)$ to be accurate for $\theta \lesssim 100°$.

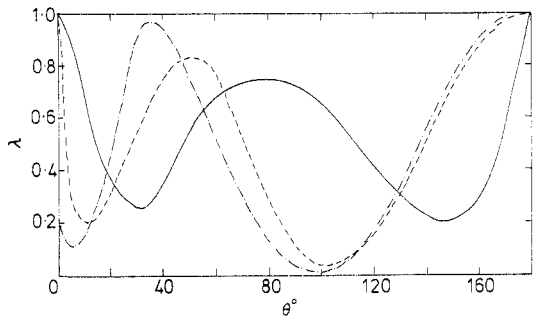

Figure 4. The ratio λ of $\sigma(M_L = 0)$ to the total differential cross section for excitation of Li (^{2}P), at selected energies in the UDWPO II approximation. —— 5·1 eV; ------ 20 eV; -·-·-·- 54·4 eV.

3.2. Sodium

3.2.1. Integral cross sections. Our results for the integrated (total) cross section for the transition

$$e^- + Na(3^2S) \rightarrow e^- + Na(3^2P)$$

are given in table 3 in both DWPO I and DWPO II models, as well as in their unitarised versions, the notation being as in table 1. The differences with and without target distortion and the effects of unitarisation are similar to those obtained for Li.

Comparison with other theoretical results and with experiment is made in figures 5 and 6. In figure 5 we show the UDWPO II results with and without core exchange, the four-state close-coupling results of Moores and Norcross (1972), the seven-state close-coupling (without exchange) results of Korff *et al* (1973) and the experimental values of Enemark and Gallagher (1972) which are normalised to the FBA at 1 keV. The optical excitation results of Zapesochnyi and Shimon (1965) lead to values for the excitation cross section lying considerably lower than those of Enemark and Gallagher at low and intermediate energies. Besides the problem of optical trapping mentioned in §3.1.1, it was suggested by Smith (Moiseiwitsch and Smith 1968) that the values of Zapesochnyi and Shimon might need to be scaled up due to a possible systematic effect resulting from an incorrect evaluation of the alkali gas density. The more recent absolute data of Zapesochnyi *et al* (1975) gives excitation cross sections lying substantially higher than those of Enemark and Gallagher at low and

Table 3. Integrated (total) cross sections (πa_0^2) for $e^- + Na(3^2S) \rightarrow e^- + Na(3^2P)$.

	DWPO I		DWPO II		DWPO II + core excitation
E(eV)	Q I	Q II	Q I	Q II	Q II
5·1	79·3	48·7	59·9	38·4	32·1
8·1	77·4	57·5	59·6	46·8	41·0
12·1	68·5	55·9	54·1	46·4	43·2
22·1	—	—	41·7	38·2	—
27·2	44·7	40·2	—	—	31·1
54·4	27·6	26·4	23·6	22·8	—
100·0	—	—	15·1	14·9	—
200·0	—	—	8·85	8·80	—

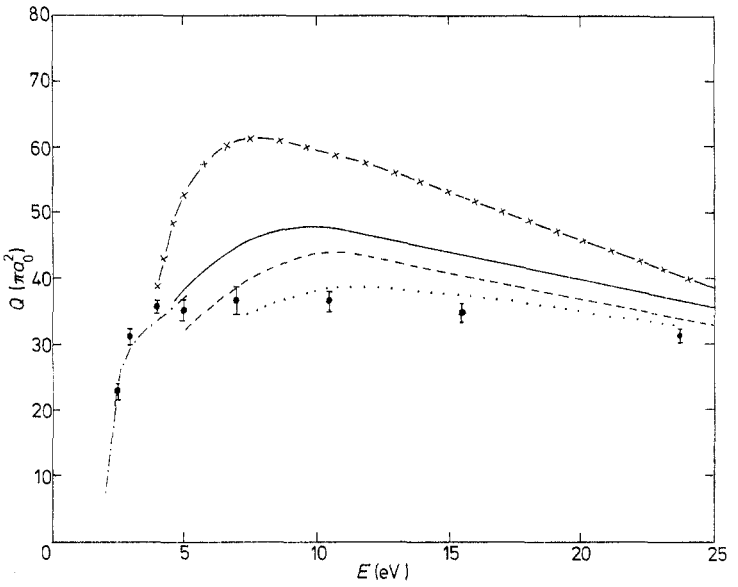

Figure 5. Integrated (total) cross sections (πa_0^2) for the resonance transition of Na from 0 to 25 eV. Experimental results: ● Enemark and Gallagher (1972); ×–×–× Zapesochnyi *et al* (1975). Theoretical results: –·–·–· four-state close-coupling (Moores and Norcross 1972); ····· seven-state close-coupling without exchange (Korff *et al* 1973); —— UDWPO II (this paper); – – – – UDWPO II including exchange with the core (this paper).

intermediate energies, but merging smoothly into the FBA at high energies; these results are also shown in figure 5. In the energy range covered by this figure, the UDWPO II results merge relatively smoothly into the four-state close-coupling calculations at about 5 eV but lie higher than the seven-state results without exchange between 7 and 23 eV; these latter values agree well with the data of Enemark and Gallagher. Though our results are reduced by about 7% at energies around 10 eV when core-exchange terms are included, they are still about 20–25% higher at the cross section maximum than the experimental values of Enemark and Gallagher, though lying well below the data of Zapesochnyi *et al* in this energy range.

Figure 6 shows the results at energies up to 1 keV in a number of theoretical models, together with the data of Enemark and Gallagher and Zapesochnyi *et al*. The FBA (Walters 1973) yields results considerably higher than the data of Enemark and Gallagher at energies below 100 eV, though it agrees well with the data of Zapesochnyi *et al* down to about ten times threshold. The Glauber calculations (Walters 1973) remain close to the experimental results of Enemark and Gallagher down to about the same energies, before beginning to underestimate the cross section. The results of McCavert and Rudge (1972) show a different energy dependence from either of the two experiments, while the UDWPO II results lie between the two experiments and merge smoothly into the data of Enemark and Gallagher at 100 eV. A two-state close-coupling calculation with an additional second-order potential in the 3s channel has been presented by Issa (1977) (see Bransden and McDowell 1978) and is in close agreement with our results. The values of Felden and Felden (1973) lie about a factor of two lower in the energy range 5–20 eV.

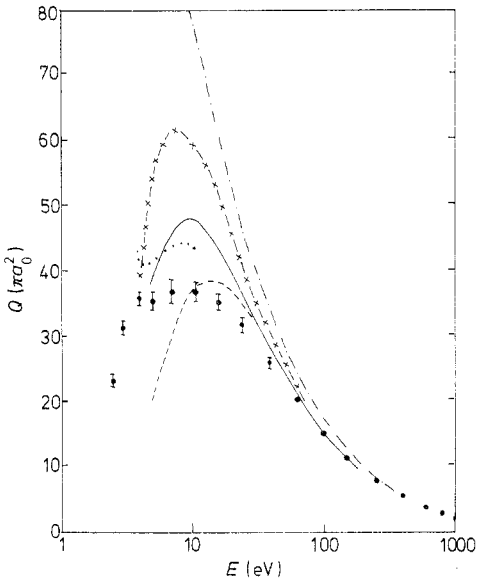

Figure 6. Integrated (total) cross sections (πa_0^2) for the resonance transition of Na to 1 keV. Experimental results: ● Enemark and Gallagher (1972); ×–×–× Zapesochnyi *et al* (1975). Theoretical results: –·–·–· FBA (Walters 1973); ––––– Glauber (Walters 1973); ····· McCavert and Rudge (1972); —— UDWPO II (this paper).

3.2.2. Differential cross sections. Calculated differential cross sections in the UDWPO II model are given in table 4 at selected energies and angles; at 5·1 eV our results are closely similar to those of Moores and Norcross (1972) at 5 eV for $\theta \leqslant 60°$. Recently, Shuttleworth *et al* (1977) have presented absolute data for the differential cross section at 54·4, 100, 150, 250 eV for values of the scattering angle less than about 20°. Our results at 54·4 and 100 eV agree very well with their values; we illustrate a comparison at 54·4 eV in figure 7. Also shown in figure 7 are the FBA and Glauber calculations (Walters 1973); the Glauber results are also consistent with the experimental data. However, in the narrow angular range over which the experimental results are available, it is not possible to make a distinction between

Table 4. UDWPO II inelastic differential cross sections ($a_0^2\,\mathrm{sr}^{-1}$) for the resonance transition of Na.

θ(deg) \ E(eV)	5·1	8·1	12·1	22·1	54·4	100
0	5·05 + 02	1·42 + 03	2·75 + 03	6·20 + 03	1·74 + 04	3·29 + 04
5	4·32 + 02	9·66 + 02	1·30 + 03	1·20 + 03	5·08 + 02	2·21 + 02
10	2·84 + 02	4·25 + 02	3·82 + 02	2·13 + 02	5·45 + 01	1·62 + 01
15	1·60 + 02	1·70 + 02	1·20 + 02	5·20 + 01	9·24 + 00	1·90 + 00
20	8·26 + 01	6·77 + 01	4·13 + 01	1·52 + 01	1·90 + 00	3·16 − 01
25	4·09 + 01	2·78 + 01	1·55 + 01	5·07 + 00	5·05 − 01	1·40 − 01
30	2·01 + 01	1·21 + 01	6·45 + 00	1·91 + 00	2·33 − 01	8·76 − 02
60	1·96 + 00	9·14 − 01	5·13 − 01	2·64 − 01	6·36 − 02	1·95 − 02
90	4·66 − 01	2·56 − 01	2·08 − 01	8·45 − 02	6·33 − 03	1·74 − 03
120	8·21 − 01	1·85 − 01	1·10 − 01	7·23 − 02	2·95 − 02	1·36 − 02
150	1·24 + 00	2·53 − 01	2·34 − 01	2·37 − 01	1·10 − 01	4·32 − 02
180	1·22 + 00	2·91 − 01	3·34 − 01	3·51 − 01	1·59 − 01	6·28 − 02

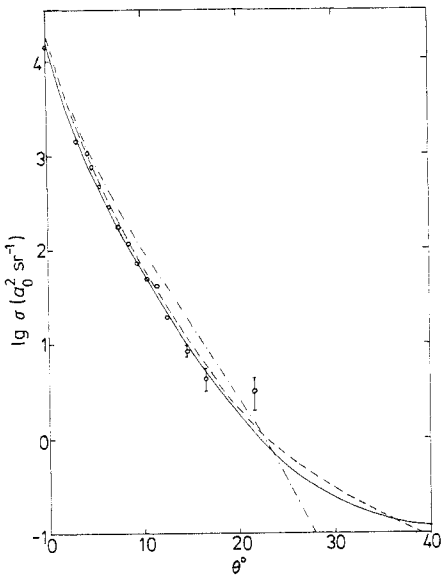

Figure 7. Differential cross sections ($a_0^2\,\mathrm{sr}^{-1}$) for the resonance transition in Na at 54·4 eV. Experimental results: ⊙ Shuttleworth *et al* (1977). Theoretical results: –·–·– FBA (Walters 1973); – – – – Glauber (Walters 1973); —— UDWPO II (this paper).

the merits of rival second-order theories which behave quite differently at larger angles. An extension of the measurements to at least 90° would be desirable. The zero-angle values tabulated by Shuttleworth *et al* are in close agreement with our values except at 150 eV where they appear to be rather low (experimental value, $(1{\cdot}33 \times 10^4 \pm 1{\cdot}4 \times 10^2)\,a_0^2\,\mathrm{sr}^{-1}$, UDWPO II value, $5{\cdot}0 \times 10^4$) which is surprising in view of the good agreement at other energies.

3.2.3. Experimental analysis of the T matrix. The time-reversed photon–electron coincidence experiment of Hertel and colleagues (Hertel 1976, Reiland 1976; see also Hermann *et al* 1977) is briefly described by Hertel, full details being given by Reiland. Na atoms in the ground state are laser excited to selective $|F, M_F\rangle$ hyperfine levels of the $^2P_{1/2}$ state and de-excited by electron collisions. The scattered electrons and emitted photons are measured in coincidence. The theory of the experiment is fully discussed by Macek and Hertel (1974). It can be interpreted as allowing a determination of various multipole moments $\langle T_{qp}^{(k)} \rangle$ of the excited Na atom, and of the ratio of the magnetic sub-level differential cross sections. These quantities follow theoretically from a knowledge of the T-matrix elements $T^{\pm}(M_L)$, for which we have available tabulated values in the UDWPO II approximation. The FBA, UDWPO II results (this paper) and close-coupling values (Moores and Norcross 1972) for $\langle T_{0+}^{(2)} \rangle$ and $\langle T_{1+}^{(2)} \rangle$ have been compared with experimental data at 5·1 eV by Reiland (1976). While at this low energy the close-coupling values lie closest to the experimental results, the UDWPO II values are a considerable improvement over the FBA. At 12·1 eV, the UDWPO II results represent a significant improvement over the FBA; no close-coupling values are available at this energy.

Fano–Macek or Stokes parameters for use in other coincidence experiments are also readily obtained from our tables of T-matrix elements. The calculated values

of λ at 54·4 eV in the UDWPO II approximation are illustrated in figure 8 and compared to the FBA results (which are independent of the wavefunctions chosen). The UDWPO II results show clear maxima and minima (cf figure 4 for Li) compared to the slowly varying FBA curve. Measurements are not yet available at this energy.

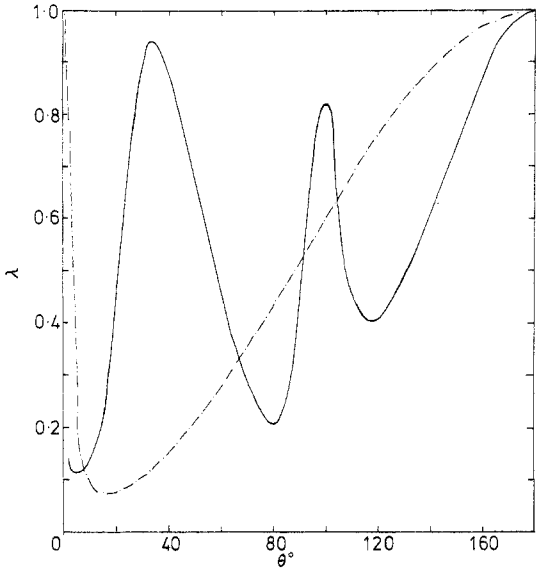

Figure 8. The ratio λ of $\sigma(M_L = 0)$ to the total differential cross section for excitation of Na (^{2}P) at 54·4 eV. Theoretical results: —— UDWPO II (this paper); –·–·–·– FBA (this paper).

3.3. Potassium

3.3.1. Integrated cross sections. Our results for the integrated (total) cross section for the transition

$$e^- + K(4^2S) \rightarrow e^- + K(4^2P)$$

are given in table 5, the notation being as in table 1. At energies below 5 eV, detailed three-state close-coupling calculations, including core polarisation, have been presented by Moores (1976); these are in reasonable agreement with the earlier two-state results of Karule and Peterkop (1965). The experimental data of Zapesochnyi and Shimon (1966), given at energies below 30 eV, is in very good agreement with the close-coupling calculations of Moores below 5 eV. However, the more recent experimental measurements of Zapesochnyi *et al* (1975), in which the optical depth of the resonance line in the atomic beam mentioned in §3.1 was taken into account, lie about 60% higher than the data of Zapesochnyi and Shimon at 5 eV. Moreover, Zapesochnyi *et al* also claim to have succeeded in checking their 1975 results for potassium by using a low-density beam, which ensured that any re-absorption was negligibly small. The experimental situation at low energies is further complicated by the recent experimental data of Williams and Trajmar (1977) who measured differential cross sections, integrated their results, and normalised the sum of the total elastic plus inelastic cross sections to the difference between the total cross sections of Kasdan *et al* (1973) and the ionisation cross sections (cf Williams *et al* 1976,

Table 5. Integrated (total) cross sections (πa_0^2) for $e^- + K(4^2S) \rightarrow e^- + K(4^2P)$ in the DWPO II model.

E(eV)	Q I	Q II
4·0	—	64·7
5·1	108	74·8
8·1	103	82·9
12·1	92·1	78·7
27·2	60·3	56·1
54·4	37·6	36·4
100·0	23·9	23·6

for Li). Williams and Trajmar estimate their uncertainties from this procedure for the excitation cross section for potassium to be $\pm 50\%$, but their results lie about a factor of two lower than those of Zapesochnyi *et al* at energies below 20 eV. This is somewhat surprising in view of the good agreement between the two corresponding experiments for Li (see §3.1). It is of interest to note that the measurements of Williams and Trajmar for K agree well with the results of Felden and Felden (1973); however, as has been pointed out in §§3.1 and 3.2, these latter calculations lie about a factor of two below other experimental and theoretical data at low energies for Li and Na. The most recent experimental and theoretical results for electron impact excitation of the resonance line of potassium at low energies are shown in figure 9. As can be seen, the UDWPO II calculations agree reasonably with the data of Zapesochnyi *et al.* However, by comparison with Li and Na, we would expect core exchange, which we have neglected, to be far more important here, and hence that our results are substantially too high at energies below 20 eV. We are inclined to believe that the only reasonably trustworthy calculations at low energies are those

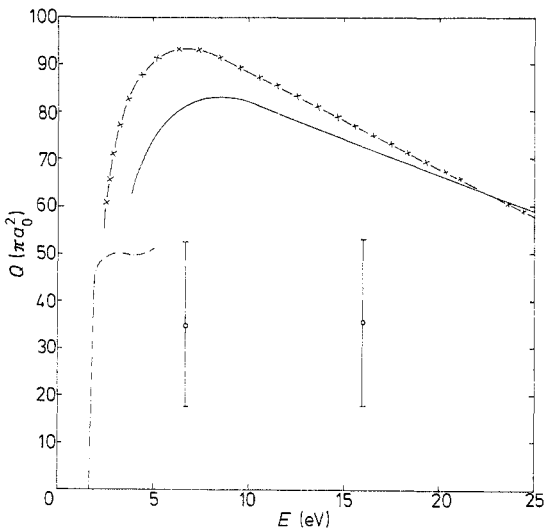

Figure 9. Integrated (total) cross sections (πa_0^2) for the resonance transition of K from 0 to 25 eV. Experimental results: ○ Williams and Trajmar (1977); ×–×–× Zapesochnyi *et al* (1975). Theoretical results: –·–·–·– three-state close-coupling (Moores 1976); —— UDWPO II (this paper).

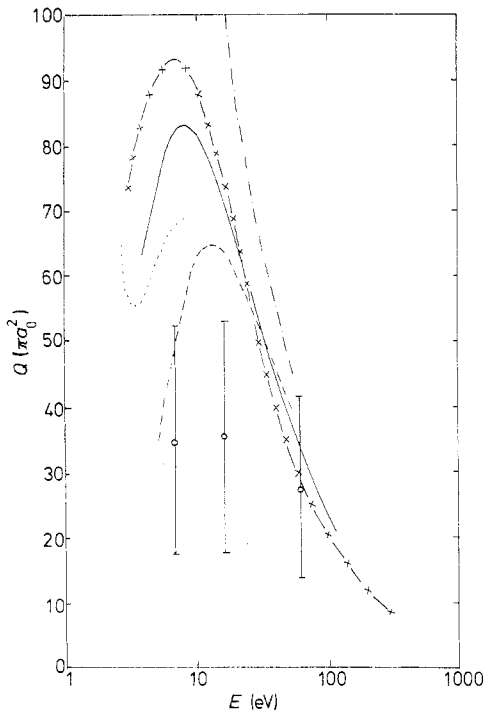

Figure 10. Integrated (total) cross sections (πa_0^2) for the resonance transition of K to 1 keV. Experimental results: ⊕ Williams and Trajmar (1977); ×–×–× Zapesochnyi *et al* (1975). Theoretical results: –·–·–·– FBA (Walters 1973); – – – – – Glauber (Walters 1973); ····· McCavert and Rudge (1972); —— UDWPO II (this paper).

of Moores (1976). There remains a serious discrepancy between the latest experiments, the reason for which is not clear at the present time.

At higher energies, the situation is perhaps less confusing. The measurements of Zapesochnyi *et al* (1975) appear to merge smoothly into the FBA at energies greater than about 300 eV, and agree well at 60 eV with the results of Williams and Trajmar (1977). In figure 10, we compare the FBA and Glauber results (Walters 1973), the UDWPO II calculations, and the values of McCavert and Rudge (1972) with the recent experimental data. As mentioned above, due to the neglect of core-exchange effects, we would expect the FBA, Glauber and UDWPO II results to be a little high at intermediate energies. As in the case of Na, the values of McCavert and Rudge show a different energy dependence from either of the two experiments.

3.3.2. Differential cross sections. Our calculated values in the UDWPO II approximations are presented in table 6. Recoil measurements are available at 5·2 eV (Slevin *et al* 1972), and our results at 5·1 eV are compared with these and the close-coupling values of Moores (1976) at 5 eV in figure 11. Allowing for the uncertainty in recoil angle in the experimental measurements, the close-coupling results are in good agreement and our values are in reasonable agreement with the experimental data for $10° \leqslant \theta \leqslant 40°$, but both theoretical approximations give a substantially larger differential cross section than the experimental result at zero angle.

Table 6. UDWPO II inelastic differential cross sections ($a_0^2\,sr^{-1}$) for the resonance transition of K.

θ(deg) \ E(eV)	5·1	8·1	12·1	27·2	54·4	100
0	1·71 + 03	4·11 + 03	7·60 + 03	2·12 + 04	4·56 + 04	8·62 + 04
5	1·30 + 03	2·20 + 03	2·47 + 03	1·51 + 03	6·52 + 02	2·62 + 02
10	6·67 + 02	7·07 + 02	5·34 + 02	1·87 + 02	5·60 + 01	1·42 + 01
15	2·92 + 02	2·25 + 02	1·40 + 02	3·80 + 01	8·28 + 00	1·61 + 00
20	1·22 + 02	7·75 + 01	4·43 + 02	1·05 + 01	1·92 + 00	5·77 − 01
25	5·06 + 01	2·96 + 01	1·67 + 01	3·98 + 00	1·01 + 00	3·46 − 01
30	2·21 + 01	1·29 + 01	7·32 + 00	2·23 + 00	7·04 − 01	2·21 − 01
60	2·60 + 00	1·23 + 00	7·54 − 01	2·31 − 01	4·11 − 02	1·51 − 02
90	8·92 − 01	4·61 − 01	2·11 − 01	2·46 − 01	1·02 − 01	3·09 − 02
120	6·57 − 01	4·61 − 01	3·60 − 01	2·05 − 01	4·70 − 02	2·81 − 03
150	8·15 − 01	1·24 + 00	1·07 + 00	6·72 − 02	7·84 − 02	7·37 − 02
180	9·34 − 01	1·79 + 00	1·51 + 00	1·36 − 01	2·15 − 01	1·33 − 01

At higher energies we may compare our UDWPO II results with the data of Williams and Trajmar (1977) over a wider range of angles. Our results at 54·4 eV are compared with their measurements at 60 eV in figure 12. There is fair agreement in shape out to 110°, but, even allowing for the uncertainties in the experimental data mentioned earlier, our results lie about a factor of two lower than the measurements for $10° \leqslant \theta \leqslant 110°$, while at zero angle, our differential cross section is an order of magnitude larger than that extrapolated by Williams and Trajmar. The situation is even less satisfactory if the inelastic differential cross section is considered as a function of energy for fixed angles (see figure 13). The comparison made in figure 12

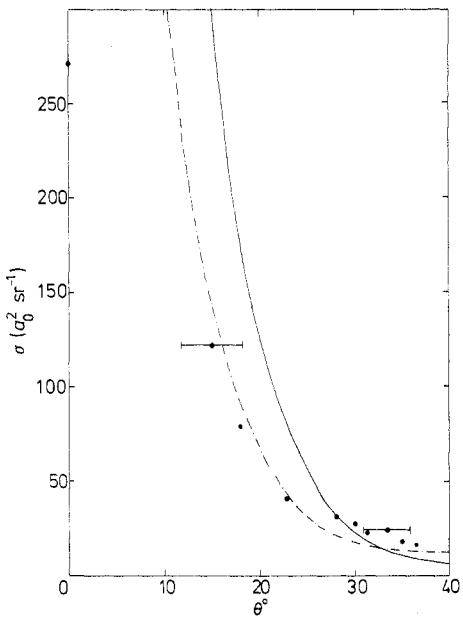

Figure 11. Differential cross sections ($a_0^2\,sr^{-1}$) for the resonance transition in K. Experimental results: ⊢●⊣ Slevin *et al* (1972) at 5·2 eV. Theoretical results: –·–·– three-state close-coupling (Moores 1976) at 5·0 eV; —— UDWPO II (this paper) at 5·1 eV.

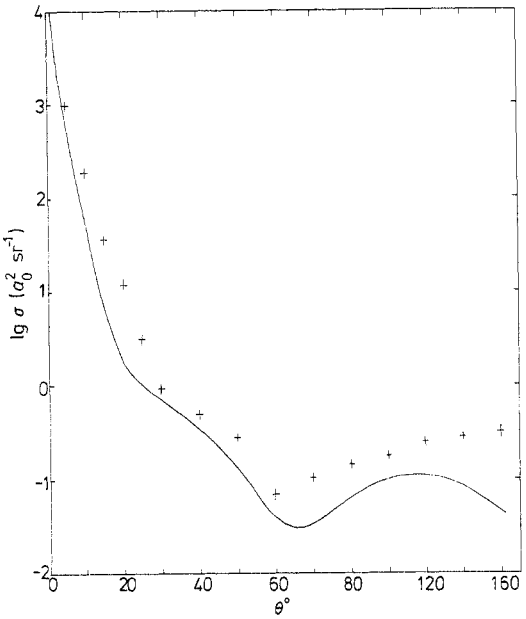

Figure 12. Differential cross sections ($a_0^2\,\mathrm{sr}^{-1}$) for the resonance transition in K. Experimental results: + Williams and Trajmar (1977) at 60 eV; the anticipated uncertainties are $\pm 50\%$. Theoretical results: —— UDWPO II (this paper) at 54·4 eV.

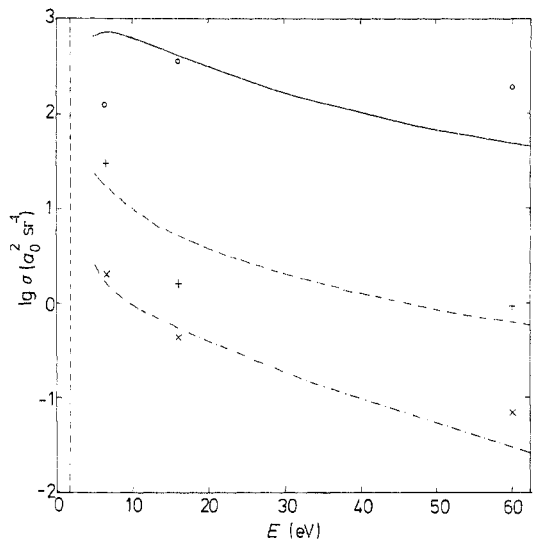

Figure 13. Differential cross sections ($a_0^2\,\mathrm{sr}^{-1}$) for the resonance transition of K at fixed scattering angles. Experimental results: Williams and Trajmar (1977), at 6·7, 16 and 60 eV; the anticipated uncertainties are $\pm 50\%$. Theoretical results: UDWPO II (this paper). $\theta = 10°$: ○ (expt); —— (theory); $\theta = 30°$: + (expt); – – – – – (theory); $\theta = 60°$: × (expt); –·–·–·– (theory).

of theoretical calculations at 54·4 eV with experimental data taken at 60 eV should therefore be viewed with some caution. For example, the calculated differential cross section at 20° drops by almost a factor of five between 27·2 and 54·4 eV, and by more than a factor of three between 54·4 and 100 eV. Interpolated values for $\theta > 5°$ at 60 eV lie further below the experimental data than shown in figure 12. The general scale of agreement of the UDWPO II results with the experimental data of Williams and Trajmar is within a factor of three almost everywhere, but substantial work remains to be done in order to obtain satisfactory convergence between theory and experiment.

3.3.3. Orientation and alignment parameters. No electron–photon coincidence experiments, or equivalent experiments, have yet been reported in the literature. However, for completeness, and as an aid to interpreting future experiments, we have available tables of our predictions, expressed (as in the case of Li and Na) as real and imaginary parts of the singlet and triplet T matrices for each angular momentum sub-state, $T^{\pm}(M_L)$. Figure 14 shows our results for the simplest parameter, λ, at three low energies; experiments to test the predicted behaviour, especially with regard to the amplitude and phase of the oscillations, would be of interest.

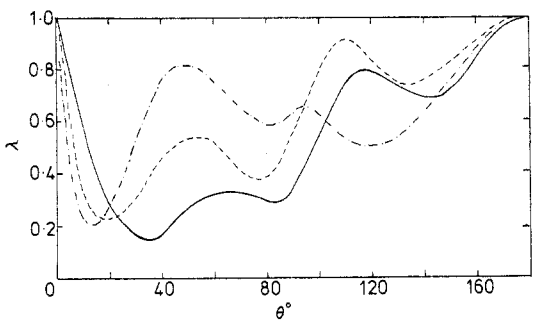

Figure 14. The ratio λ of $\sigma(M_L = 0)$ to the total differential cross section for excitation of K (^{2}P) at selected energies in the UDWPO II approximation. —— 5·1 eV; – – – – 8·1 eV; –·–·–·– 12·1 eV.

3.3.4. Spin-flip differential cross sections. The atomic-beam recoil technique has been used by Goldstein *et al* (1972) to obtain the ratio, $R(\theta)$, of the spin-flip differential cross section to the total differential cross section for excitation of the resonance transition in potassium. The experiment uses spin-polarised atoms and unpolarised electrons and measures the proportion of atoms which spin-flip after electron impact excitation to the 4p state and subsequently decay back to the 4s state. The derivation of the appropriate expression for $R(\theta)$ in terms of T-matrix elements has been given by Rubin *et al* (1969) and Moores and Norcross (1972). Figure 15 illustrates the results for $R(\theta)$ for potassium obtained from our UDWPO II model and the three-state close-coupling calculations of Moores (1976), together with the experimental values of Goldstein *et al* (1972). At 5 eV, the close-coupling calculations agree more closely with the experimental measurements, although the shape of our curve at 5·1 eV is similar, but both theories give values higher than experiment at small angles ($< 10°$). At 8·1 eV, our curve lies about 15% above experiment at 8 eV for $5 \leqslant \theta \leqslant 15°$ but is 22% higher at $\theta = 0°$, while at larger angles ($\theta > 15°$) our values begin to increase

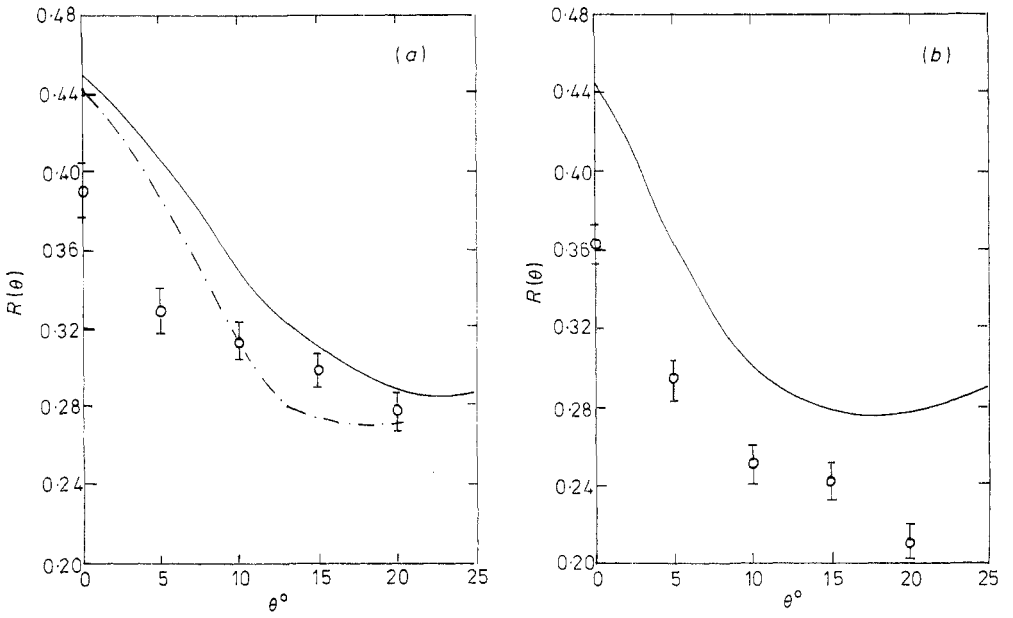

Figure 15. The ratio $R(\theta)$ of the spin-flip cross section to the total differential cross section for excitation of K (^{2}P). (*a*) ⊖ experimental results (Goldstein *et al* 1972) at 5 eV; –·–·– three-state close-coupling (Moores 1976) at 5 eV; —— UDWPO II (this paper) at 5·1 eV. (*b*) ⊖ experimental results (Goldstein *et al* 1972) at 8 eV; —— UDWPO II (this paper) at 8·1 eV.

whereas experiment continues to decrease. The minimum we predict at 8·1 eV is seen in the experimental data at 7, 9 and 10 eV (not shown), but not at 8 eV. Further work is clearly desirable.

4. Conclusion

We have extended our distorted-wave polarised-orbital approximation to study the resonance transitions in alkali metals at intermediate energies above the ionisation threshold. The results for the total (integrated) inelastic cross sections for excitation of these transitions in Li, Na and K appear to be in at least as good agreement with experiment as the Glauber results, if the JILA measurements are taken as standard, and in rather better agreement with the recent Russian work. They are in fair agreement with available close-coupling calculations at low energies, but must be considered less reliable than these. We feel that our differential cross sections are reasonably reliable for scattering angles up to 100° and we have available tables of T-matrix elements for use in the analysis of electron–photon coincidence experiments.

It is clear that much more work, both theoretical and experimental, is required in the intermediate energy region in order to resolve the anomalies pointed out in §3. Walters (1976) suggested that renormalisation of the total experimental cross sections of Kasdan *et al* (1971) for Li by a factor of 0·76 would reduce the experimental excitation data of Williams *et al* (1976) by about the same amount, placing their

points at 5·4, 10 and 20 eV about 10% below the results of Leep and Gallagher (1974) and their point at 60 eV about 20% higher than that of Leep and Gallagher. The data of Zapesochnyi *et al* (1975) agree well with the present results of Williams *et al*, but lies about 18% higher than the values of Leep and Gallagher in the range 5–20 eV. The close-coupling calculations of Burke and Taylor (1969) give values slightly above the present experimental values in this energy range, while our UDWPO II results are closer to those of Williams *et al*. A similar situation occurs for Na; the data of Zapesochnyi *et al* (1975) lies between 45 and 60% higher than that of Enemark and Gallagher (1972) for excitation of the ^{2}P state in the range 5–20 eV. The four-state close-coupling calculations of Moores and Norcross (1972) agree well with the values of Enemark and Gallagher below 5 eV, while our UDWPO II results lie between the two experiments in the range 5–20 eV, but are closer to the data of Enemark and Gallagher. For K, the situation is considerably worse. Here the experimental results of Williams and Trajmar (1977), obtained in precisely the same manner as their data for the excitation of the ^{2}P state of Li, lie considerably more than a factor of two lower than the values of Zapesochnyi *et al* (1975) for excitation of the ^{2}P state in the range 5–20 eV. The three-state close-coupling results of Moores (1976) agree well with the earlier data of Zapesochnyi and Shimon (1966) below 5 eV, while our UDWPO II calculations lie slightly lower than the data of Zapesochnyi *et al* in the range 5–20 eV. Clearly, substantial improvements, such as the inclusion of core effects, are needed in the theoretical models at intermediate energies for potassium, together with further data to resolve the experimental anomalies.

Acknowledgments

One of us (JVK) is indebted to the Science Research Council for a studentship. We are all grateful to our experimental colleagues for many fruitful discussions, and particularly to Dr I V Hertel, Dr S Trajmar and Mr T Shuttleworth, who provided experimental data prior to publication.

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