Electron impact excitation of the 3^2D states of lithium, sodium and potassium atoms

Surbhi Verma and Rajesh Srivastava

Department of Physics, University of Roorkee, Roorkee 247 667, India

Abstract. A systematic study of the electron impact 3^2D excitation of lithium, sodium and potassium from their ground states is considered in distorted-wave approximation theory. Results for differential and integrated cross sections, alignment, orientation and spin asymmetry parameters in the energy range 10–100 eV are calculated and presented. Our integrated cross section results show good agreement when compared with other theories and available experiments. Present differential cross section results for sodium are also compared with the only available recent differential cross section measurements. For the sake of further meaningful comparison and discussions, the first Born calculations for the cross sections are also performed and compared.

1. Introduction

Most of the previous investigations of electron impact excitation of atoms have considered the excitations of atoms from their ground states to the excited higher S and (or) P states which involve transfer of zero or one unit of angular momentum. Thus, such excitations are fairly well studied and there are various theoretical and experimental studies available. For example, for hydrogen, helium, alkali and other atoms, see the reviews of Andersen *et al* (1988), Slevin and Chwirot (1990), Becker *et al* (1992) and references therein. These studies have reported differential and integrated cross sections for S and P excitations as well as alignment and orientation parameters for the excited P states. In contrast, comparatively little similar work has been devoted so far to the equally important and more interesting phenomenon of electron excitation of the excited D states of atoms where transfer of two units of angular momentum is involved. The main reason has obviously been the small excitation cross sections and the complexity involved in dealing with such excitations. In particular, it is relatively difficult experimentally to resolve an excited D state from its magnetic substates as well as from other overlapping excited states.

However, experiments with electron–photon angular and polarization correlation techniques will now allow us to study individual D states, basically because of the fact that photons from the decay of the excited D states can be readily isolated. Consequently, during the recent past some theoretical and experimental studies in this light have become available for hydrogen and helium, dealing with the orientation and alignment results for the excitation of the 3D states (Williams and Wang 1994 and references therein, Mikosza *et al* 1994, Crowe *et al* 1994, Bray *et al* 1995, Verma and Srivastava 1995a). It should be emphasized that the lighter alkalis, namely Li, Na and K are the next most studied atoms after hydrogen and helium where similar studies can be easily extended. From this

viewpoint as well as a continuation to our previous theoretical work on 3D excitation of hydrogen and helium (Katiyar and Srivastava 1987, 1989, Farrell *et al* 1990, Verma and Srivastava 1995a) we extend in the present paper our similar systematic and complete study to the electron excitation of the excited 3^2D states from the ground n^2S state of Li ($n = 2$), Na ($n = 3$) and K ($n = 4$). We hope that our present effort will stimulate more theoretical and experimental work and may be useful as a guide for experimentalists.

We find that most of the earlier theoretical and/or experimental studies on electron impact 3^2D excitation from the ground states of Li, Na and K have reported only integrated cross sections. These include the experimental data of Zajonc and Gallagher (1979) for lithium and Stumpf and Gallagher (1985) for sodium. Theoretical calculations were made using the first Born approximation (see Moiseiwitsch and Smith 1968) for Li, Na and K, the close coupling results of Msezane (1988) for Na as well as the unitarized distorted-wave results of Mitroy (1993) and close coupling results of Msezane *et al* (1992) for K. However, for differential cross section (DCS) results it is only very recently that Marinkovic′ *et al* (1992) have reported their first measurement on 3^2D excitation in the sodium atom. Except for this work no other theoretical and experimental DCS results are available for any of the lighter Li, Na and K alkalis.

It has been realized over the years that a distorted-wave approximation (DWA) is quite suitable for the calculation of cross sections and angular correlation parameters and gives reliable results (Slevin and Chwirot 1990, Itikawa 1986). For electron impact excitation of atoms at intermediate and high energies, unlike close-coupling type calculations the DWA does not suffer from any convergence problem at such energies. We have therefore considered in the present paper the electron impact 3^2D excitation in Li, Na and K in the framework of a DWA theory. Our DWA method used here is an extension of the method which we used recently for studying 3^2S–3^2P excitation in Na and 4^2S–4^2P, 5^2P excitations in K (Verma and Srivastava 1995b, 1996). We have carried out calculations for all parameters which one would need to completely describe the collision process. These results are presented and compared with experiment and other theories where available.

2. Theoretical considerations (DWA theory)

2.1. Differential and integrated cross sections

For the present study the alkali atoms (namely Li, Na and K) are treated as one-electron systems and the effect of the core electrons is incorporated in the form of a core potential. The T-matrices in the distorted-wave approximation for the electron impact excitation of an alkali atom from an initial ground state 'i' to a final state 'f' (with magnetic quantum number 'm') in the singlet (s) or triplet (t) mode can be expressed in the 'collision frame of reference' as

$$T_m^{s(t)} = T_m^d \pm T_m^{ex}. \tag{1}$$

The $+$ ($-$) sign is associated with the scattering in the singlet (triplet) mode. Further, the spin-averaged direct (T_m^d) and exchange (T_m^{ex}) T-matrices are given by

$$T_m^d = \langle F^-(\mathbf{k}_f, 2)\phi_{f_m}(1)|V(1, 2) - U_f(2)|\phi_i(1)F^+(\mathbf{k}_i, 2)\rangle \tag{2}$$

$$T_m^{ex} = \langle F^-(\mathbf{k}_f, 2)\phi_{f_m}(1)|V(1, 2) - U_f(2)|\phi_i(2)F^+(\mathbf{k}_i, 1)\rangle. \tag{3}$$

Here, V is the total interaction potential between the target alkali atom and the projectile electron expressed by (atomic units are used throughout)

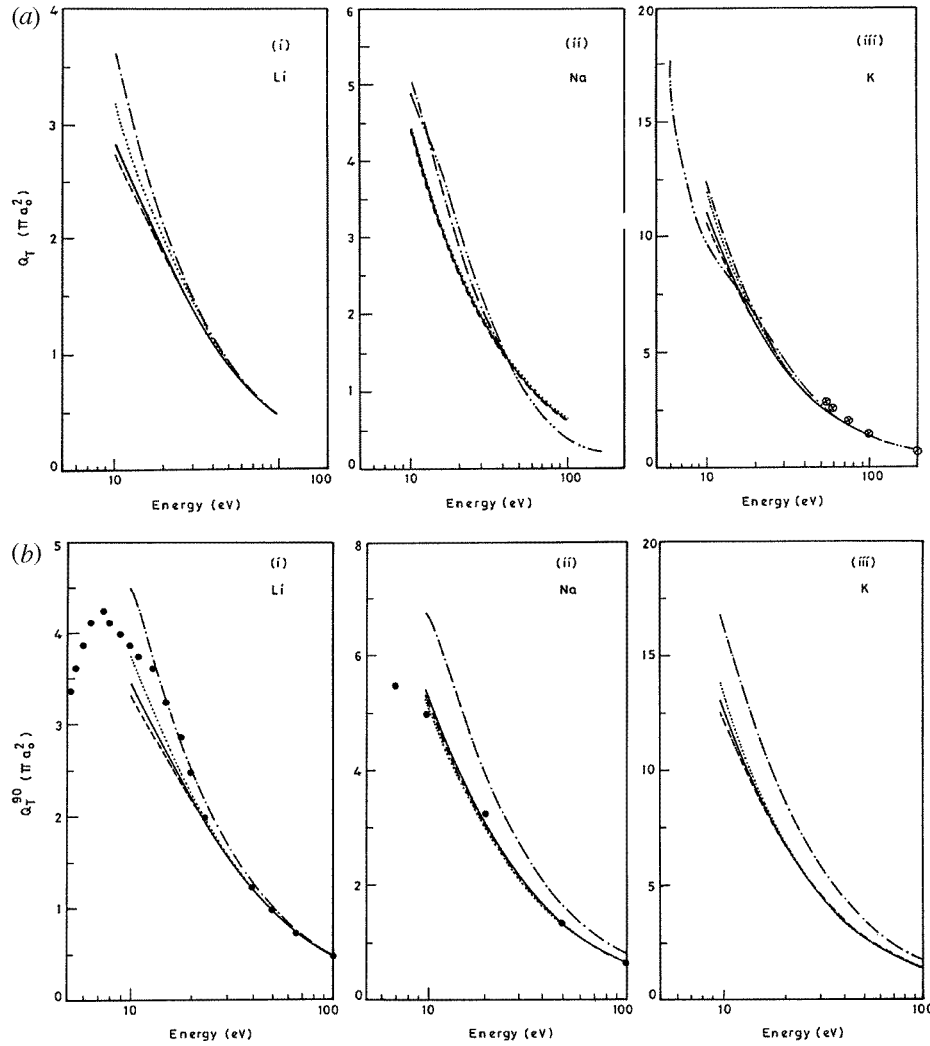$$V = -\frac{1}{r_2} + \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} + V^{core}(r_2) \tag{4}$$

Figure 1. (*a*) Total cross section Q_T in units of πa_0^2 for 3^2D excitation in Li, Na and K. ——, present FF results; ······, present IF results; – – –, present IIP results; — · —, present FBA results; — · · —, 4CC results for Msezane *et al* (1988) for Na and 7CC results of Msezane (1992) for K; ○ , UBA results of Mitroy (1992) for K; ×, UDWBA results of Mitroy (1992) for K. (*b*) As (*a*) except for Q_T^{90} and ● , experimental data of Zajonc and Gallagher (1979) for Li and experimental data of Stumpf and Gallagher (1985) for Na.

where r_1 and r_2 are the position coordinates of the target and projectile electrons, respectively, with respect to the target nucleus. Further, the core potential, V^{core}, of the target alkali atom is given by

$$V^{core} = \sum_{n=1}^{j} N_{nl} \int \frac{|R_{nl}(r)|^2 r^2 \, dr}{r_>} \tag{5}$$

where $j = 1, 2, 3$ for lithium, sodium and potassium, respectively. N_{nl} represents the occupation number of the electrons in different orbitals referred to by n and l quantum numbers and R_{nl} is the corresponding radial wavefunction.
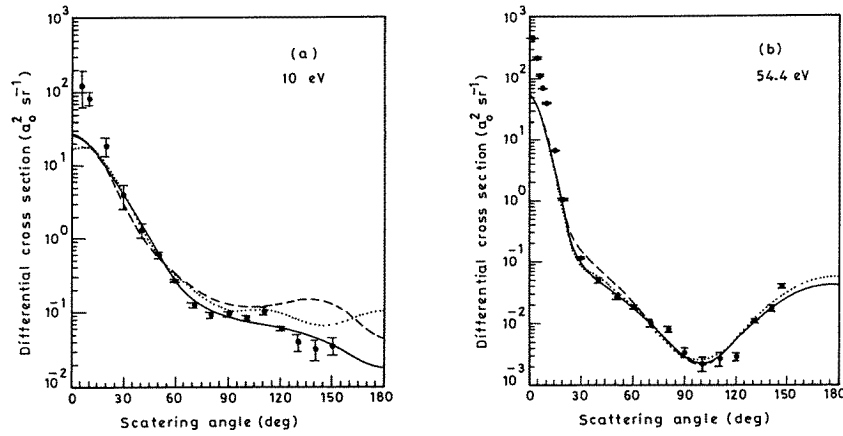
Figure 2. Differential cross section in units of $a_0^2 \text{sr}^{-1}$ for the 3^2S–3^2D excitation in Na at an electron impact energy of (*a*) 10 eV and (*b*) 54.4 eV. ——, present FF results; $\cdots\cdots$, present IF results; $---$, present IIP results; ● , experimental data of Marinkovic´ *et al* (1992).

$\phi_{i(f)}$ is the initial (final) state wavefunction of the target atom. These are represented in terms of Hartree–Fock wavefunctions. For lithium and sodium ϕ_i is taken from Szasz and McGinn (1967) and ϕ_f from Daniele (1979, 1980), while for potassium both ϕ_i and ϕ_f are taken from Mitroy (1993). $F_{i(f)}^{+(-)}$ represents the initial (final) channel projectile distorted wave with the wavevector $\mathbf{k}_i$ ($\mathbf{k}_f$) and the associated superscript $+(-)$ indicates the usual outgoing (incoming) wave boundary conditions. These are the solutions of the following equation:

$$(\nabla^2 + k_j^2 - 2U_j)F^{\pm}(\mathbf{k}_j, \mathbf{r}) = 0 \qquad \text{with } j = i \text{ or } f. \tag{6}$$

$U_{i(f)}$ is the distortion potential in the initial (final) channel. This is taken to be, as in our previous work (Verma and Srivastava 1995b), the sum of the spherically averaged static potential, exchange potential and polarization potential, i.e.

$$U_j = V_j^{\text{stat}} + V_j^{\text{ex}} + V_j^{\text{pol}} \tag{7}$$

with static potential

$$V_j^{\text{stat}} = \langle \phi_j | V | \phi_j \rangle \qquad (j = i \text{ or } f). \tag{8}$$

For the exchange potential, V_j^{ex}, the following most widely used form as given by Furness and McCarthy (1973) is taken:

$$V_j^{\text{ex}} = \tfrac{1}{2} \left\{ (\tfrac{1}{2}k_j^2 - V_j^{\text{stat}}) - [(\tfrac{1}{2}k_j^2 - V_j^{\text{stat}})^2 - 8\pi\tau\rho_j]^{1/2} \right\} \tag{9}$$

where ρ_j is the spherically averaged charge density of the alkali atom in the initial or final channel and τ is taken to be $+1$ (-1) for scattering in the singlet (triplet) mode of the system (Vučic´ *et al* 1987).

Further, V_j^{pol} is the polarization potential and is chosen to be of the Buckingham type, as proposed by Jhanwar and Khare (1976)

$$V_j^{\text{pol}} = -\frac{\alpha_d r^2}{2(r^2 + d^2)^3}. \tag{10}$$

Here α_d is the static dipole polarizability of the atom and may be obtained as available in the literature (see Miller and Bederson 1977). The value of d is chosen, as suggested by Mittleman and Watson (1960), as having the following form

$$d = (\tfrac{1}{2}\alpha_d\beta^2 Z^{-1/3})^{1/4} \tag{11}$$

where Z is the nuclear charge of the target alkali atom and β, the energy-dependent parameter, is taken to be unity in the present calculation, i.e. energy independent.
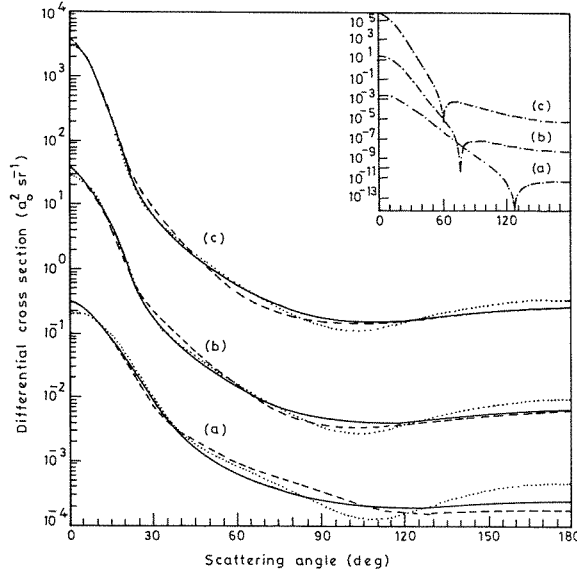

Figure 3. Differential cross section in units of $a_0^2\text{sr}^{-1}$ for the 2^2S–3^2D excitation in Li at (*a*) 20 eV, (*b*) 40 eV and (*c*) 60 eV. ——, present FF results; ······, present IF results; - - - -, present IIP results; — · —, present FBA results. Each FF, IF and IIP DWA result at 20 and 60 eV has been multiplied by a factor of 0.01 and 100 respectively while the corresponding FBA results are multiplied by 0.0001 and 10 000, respectively.

In principle, in the distorted wave approximation the distortion potential U_j in the initial or final channel may be chosen in any suitable arbitrary manner (Madison *et al* 1991, Verma and Srivastava 1994). As seen from previous applications (Verma and Srivastava 1995a, b, Verma *et al* 1995) of DWA theory, if the distortion potential of the excited state static and exchange potentials is taken in both the initial and final channels (referred to as FF model) it explains experimental results in the best way. The same choice is therefore adopted for our calculations. In addition, we carried out calculations with two further choices. First, by using the traditional Mott–Massey (1965) version where the initial and final channel distortion potentials are taken of the initial and final excited state static and exchange potential respectively (IF model). Second, by using ground state static, exchange and polarization potentials in both channels to see the effect of polarization. This choice of considering polarization through the ground state is due to availability of accurate dipole polarizability only for the ground n^2S states of alkali atoms. Here we have taken $\alpha_d = 164$, 159, 293 respectively for Li, Na and K atoms (see Miller and Bederson 1977). As earlier, we refer to this choice as our IIP model. Thus in this paper we will present our results in the FF, IF and IIP models.

After the distortion potentials are defined, we expand the distorted waves F^+ and F^- using the following general form of partial wave expansion

$$F^{+(-)}(\mathbf{k}, \mathbf{r}) = \frac{1}{\sqrt{k}} \sum_{\ell=0}^{\infty} (2\ell + 1) i^\ell e^{\pm i\delta_\ell(k^2)} \frac{u_\ell^\pm(k, r)}{r} P_\ell(\hat{\mathbf{k}} \cdot \hat{\mathbf{r}}) \qquad (12)$$

where δ_ℓ is the phase shift of the ℓth partial wave, P_ℓ is Legendre polynomial of order ℓ and $u_\ell^\pm(k, r)$ is the radial part of the distorted wave. On substituting $F^\pm$ as given above in equation (6) we get

$$\left[\frac{d^2}{dr^2} + k^2 - \frac{\ell(\ell + 1)}{r^2} + 2U(r) \right] u_\ell(k, r) = 0 \qquad (13)$$

which is solved numerically subject to the following usual boundary conditions

$$u_\ell(k, r) \underset{r \to 0}{=} 0 \qquad (14a)$$

and

$$u_\ell(k, r) \underset{r \to \infty}{=} \frac{1}{\sqrt{k}} \sin[kr - \tfrac{1}{2}\ell\pi + \delta_\ell(k^2)]. \qquad (14b)$$

As adopted in our previous various calculations, the numerical integration of the radial equation (13) is done using Numerov's method. However, to start the solution near the origin a power series solution is used. The radial mesh is determined by the nuclear charge Z and we have used a different radial mesh size (Δr) and maximum radius (r_{max}) for each of the alkali atoms. The respective adopted values for the Li, Na and K atoms for ($\Delta r, r_{max}$) are (1.54×10^{-3}, 125.69), (9.95×10^{-4}, 81.47) and (8.29×10^{-4}, 67.87).
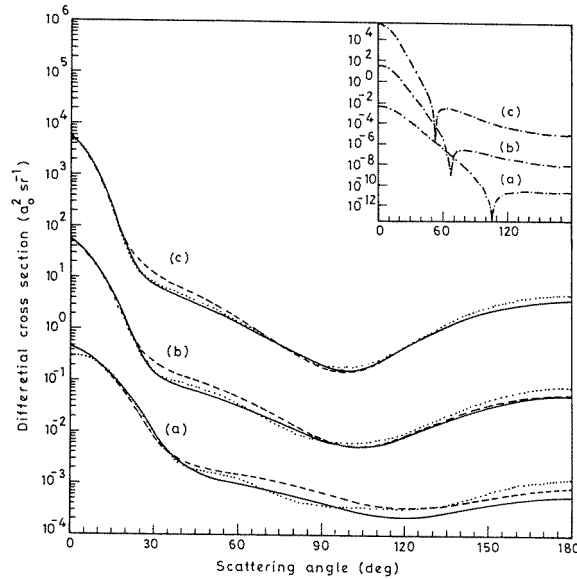

Figure 4. Same as figure 3 but for the 3^2S–3^2D excitation in Na.

Finally, the direct and exchange T-matrices (equations (2) and (3)) are evaluated for excitation of each magnetic substate of the excited D state. First, we simplify the expressions by carrying out the straightforward but lengthy standard angular momentum algebra for angular integration and then perform the radial integrations using Simpson's method. We
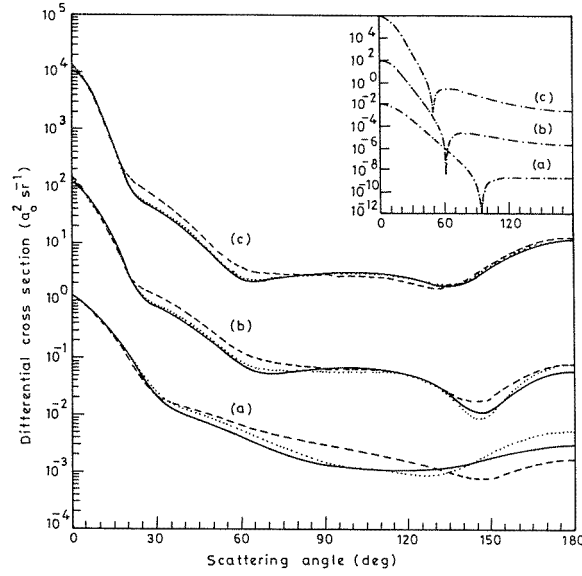
Figure 5. Same as figure 3 but for the 4^2S–3^2D excitation in K.

Table 1. Comparison of results for Q_T^{90} (units of πa_0^2) for the 2^2S–3^2D excitation in Li.

Energy (eV)	Present results				Experiment (Zajonc *et al* 1979)
	FF	IF	IIP	FBA	
5	—	—	—	—	3.00(+00)
10	3.49(+00)	3.77(+00)	3.30(+00)	4.52(+00)	3.88(+00)
15	2.73(+00)	2.85(+00)	2.66(+00)	3.30(+00)	3.25(+00)
20	2.22(+00)	2.27(+00)	2.19(+00)	2.55(+00)	2.50(+00)
25	1.86(+00)	1.89(+00)	1.85(+00)	2.06(+00)	2.00(+00)
30	1.59(+00)	1.61(+00)	1.59(+00)	1.72(+00)	—
40	1.23(+00)	1.23(+00)	1.23(+00)	1.29(+00)	1.25(+00)
50	9.90(−01)	9.90(−01)	9.96(−01)	1.03(+00)	1.00(+00)
60	8.32(−01)	8.31(−01)	8.34(−01)	8.58(−01)	—
70	7.16(−01)	7.13(−01)	7.16(−01)	7.33(−01)	—
80	6.27(−01)	6.24(−01)	6.28(−01)	6.39(−01)	—
90	5.57(−01)	5.55(−01)	5.58(−01)	5.67(−01)	—
100	4.99(−01)	4.99(−01)	5.02(−01)	5.09(−01)	5.00(−01)

obtain the T-matrices for the singlet and triplet modes separately. Since in the present paper we have considered only the excitation of the S state to a D state which is optically forbidden (unlike S–P excitation), we did not face any convergence problem over the summation of the partial waves of the scattered electron in evaluating the T-matrices. We found the maximum value of the partial waves required for the convergence of the T-matrices increased with the incident electron energy. For example, it was nearly 250 at 100 eV to achieve convergence to an accuracy of 10^{-6} for the direct T-matrix.

Table 2. Comparison of results for Q_T^{90} (units of πa_0^2) for the 3^2S–3^2D excitation in Na.

Energy (eV)	Present results				Experiment (Stumpf *et al* 1985)
	FF	IF	IIP	FBA	
5	—	—	—	—	5.10(+00)
10	5.54(+00)	5.41(+00)	5.45(+00)	6.76(+00)	5.00(+00)
15	3.86(+00)	3.73(+00)	3.79(+00)	5.07(+00)	—
20	3.08(+00)	3.02(+00)	3.06(+00)	3.99(+00)	3.27(+00)
25	2.56(+00)	2.51(+00)	2.56(+00)	3.28(+00)	—
30	2.17(+00)	2.15(+00)	2.19(+00)	2.78(+00)	—
40	1.67(+00)	1.65(+00)	1.68(+00)	2.11(+00)	—
50	1.35(+00)	1.34(+00)	1.36(+00)	1.70(+00)	1.37(+00)
60	1.13(+00)	1.12(+00)	1.14(+00)	1.42(+00)	—
70	9.70(−01)	9.67(−01)	9.79(−01)	1.22(+00)	—
80	8.49(−01)	8.46(−01)	8.56(−01)	1.07(+00)	—
90	7.55(−01)	7.45(−01)	7.60(−01)	9.49(−01)	—
100	6.99(−01)	6.92(−01)	6.84(−01)	8.53(−01)	6.50(−01)

Table 3. Comparison of results for Q_T^{90} (units of πa_0^2) for the 4^2S–3^2D excitation in K.

Energy (eV)	Present results			
	FF	IF	IIP	FBA
10	12.98(+00)	13.64(+00)	12.35(+00)	16.55(+00)
15	8.95(+00)	9.26(+00)	8.97(+00)	11.63(+00)
20	6.96(+00)	7.12(+00)	6.99(+00)	8.89(+00)
25	5.65(+00)	5.70(+00)	5.69(+00)	7.18(+00)
30	4.72(+00)	4.73(+00)	4.78(+00)	6.01(+00)
40	3.54(+00)	3.52(+00)	3.61(+00)	4.52(+00)
50	2.83(+00)	2.82(+00)	2.89(+00)	3.61(+00)
60	2.36(+00)	2.35(+00)	2.41(+00)	3.00(+00)
70	2.02(+00)	2.02(+00)	2.06(+00)	2.57(+00)
80	1.77(+00)	1.77(+00)	1.80(+00)	2.24(+00)
90	1.58(+00)	1.54(+00)	1.59(+00)	1.99(+00)
100	1.42(+00)	1.41(+00)	1.44(+00)	1.79(+00)

Further, the scattering amplitude for each magnetic substate (with $m = 0, \pm 1, \pm 2$) of the final 3^2D state of Li, Na and K is related to the T-matrix by

$$a_m^{s(t)} = -\frac{1}{2\pi} T_m^{s(t)}. \tag{15}$$

The differential cross section (DCS) in the singlet (triplet) mode can therefore be expressed in terms of the scattering amplitude as

$$\sigma_m^{s(t)} = \frac{k_f}{k_i} |a_m^{s(t)}|^2 \tag{16}$$

and the spin-averaged DCS as

$$\sigma_m = \tfrac{1}{4}\sigma_m^s + \tfrac{3}{4}\sigma_m^t. \tag{17}$$

Finally the DCS summed over the different values of m is

$$\sigma_T = \sigma_0 + 2\sigma_1 + 2\sigma_2. \tag{18}$$

In addition, the integrated cross sections after integrating over all scattering angles for different values of m are obtained in terms of the spin-averaged DCS by

$$Q_m = \int \sigma_m \, d\Omega \tag{19}$$

and the total integrated cross section summed over all values of m by

$$Q_T = \int \sigma_T \, d\Omega. \tag{20}$$

Very often the experimentalists measure the total cross sections at 90° to the incident electron beam direction, which can be defined in terms of the total cross section Q_T by

$$Q_T^{90} = Q_T \left(\frac{3}{3 - P} \right) \tag{21}$$

where P is the polarization fraction for the radiation lines emitted by the alkali atoms following electron excitation to the 3^2D states and is expressed as

$$P = \frac{I_\parallel - I_\perp}{I_\parallel + I_\perp}. \tag{22}$$

Here $I_\parallel$ and $I_\perp$ are the intensities, observed at 90° to the incident electron beam direction, of the lines having electric vectors parallel and perpendicular to the incident beam direction, respectively. The polarization fraction for the de-excitation of the excited 3^2D state to the lower ^{2}P states of the Li, Na and K atoms, as given by Percival and Seaton (1958), can be expressed in terms of integrated cross sections as

$$P = \frac{Q_0 + Q_1 - 2Q_2}{2.07 Q_0 + 3.8 Q_1 + 2.8 Q_2}. \tag{23}$$

2.2. Stokes parameters, alignment and orientation and asymmetry parameters

For the light emitted from the decay of the excited 3^2D states of Li, Na and K, the usual Stokes parameters P_i ($i = 1, 2, 3$) measured perpendicular to the scattering plane ($\phi = 90°$) are defined as (Andersen *et al* 1988)

$$P_1 = \frac{I(0°) - I(90°)}{I(0°) + I(90°)} \tag{24a}$$

$$P_2 = \frac{I(45°) - I(135°)}{I(45°) + I(135°)} \tag{24b}$$

$$P_3 = \frac{I(\text{RHC}) - I(\text{LHC})}{I(\text{RHC}) + I(\text{LHC})}. \tag{24c}$$

Further, the Stokes parameter P_4 measured parallel to the scattering plane ($\phi = 0°$) is given by

$$P_4 = \frac{I(0°) - I(90°)}{I(0°) + I(90°)}. \tag{24d}$$

Here $I(\theta)$ is the intensity of light with the polarization vector in the θ direction with respect to the incident electron direction and $I(\text{RHC})$ and $I(\text{LHC})$ are the intensities of the right and left circularly polarized light components, respectively.
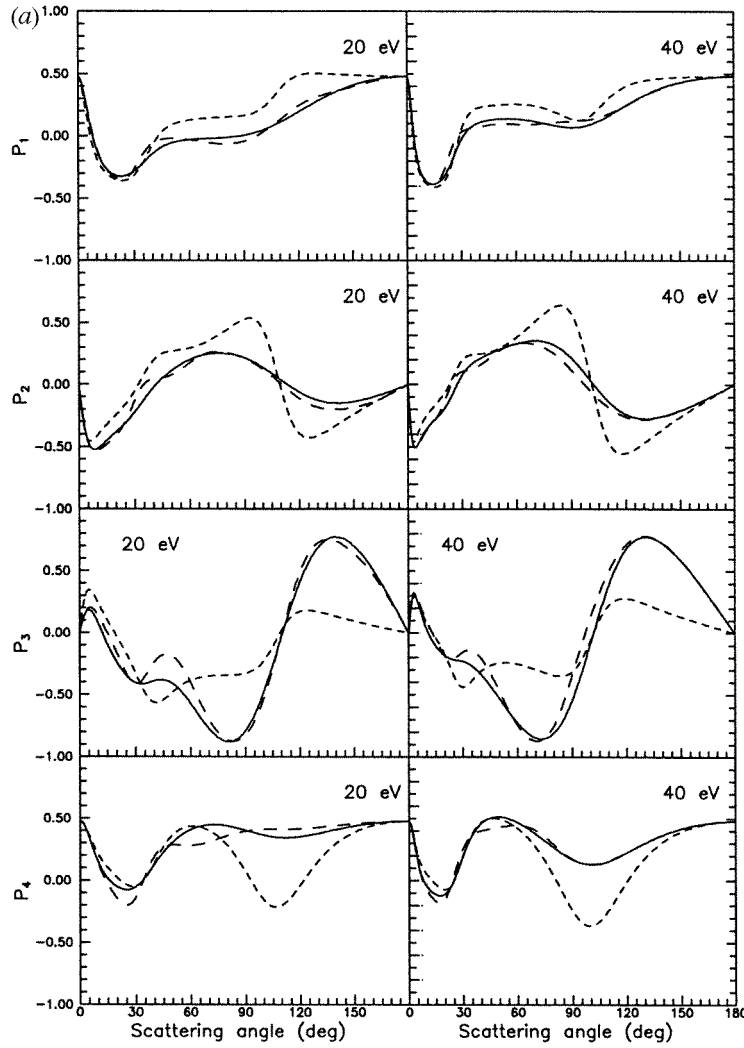
Figure 6. (*a*) Stokes parameters P_1–P_4 for the 2^2S–3^2D excitation in Li at 20 and 40 eV. Symbols: the same as figure 3. (*b*) As (*a*) but for coherence parameters $L_\perp$, P_l, ρ_{00} and γ. (*c*) As (*a*) but for $L_\perp^s$, $L_\perp^t$, A and r.

The Stokes parameters P_i ($i = 1$–4) can be expressed in terms of scattering amplitudes a'_m in the 'natural coordinate frame' separately for each singlet and triplet scattering mode by

$$I^z P_1 = -\frac{19}{25}(\tfrac{2}{3})^{1/2}[\mathrm{Re}(a'_0 a'^*_2) + \mathrm{Re}(a'_0 a'^*_{-2})] \tag{25a}$$

$$I^z P_2 = -\frac{19}{25}(\tfrac{2}{3})^{1/2}[\mathrm{Im}(a'_0 a'^*_2) - \mathrm{Im}(a'_0 a'^*_{-2})] \tag{25b}$$

$$I^z P_3 = -\frac{23}{25}(|a'_2|^2 - |a'_{-2}|^2) \tag{25c}$$

$$I^y P_4 = \frac{19}{50}[1 - 2|a'_0|^2 - (\tfrac{2}{3})^{1/2}(\mathrm{Re}(a'_0 a'^*_2) + \mathrm{Re}(a'_0 a'^*_{-2}))] \tag{25d}$$

where

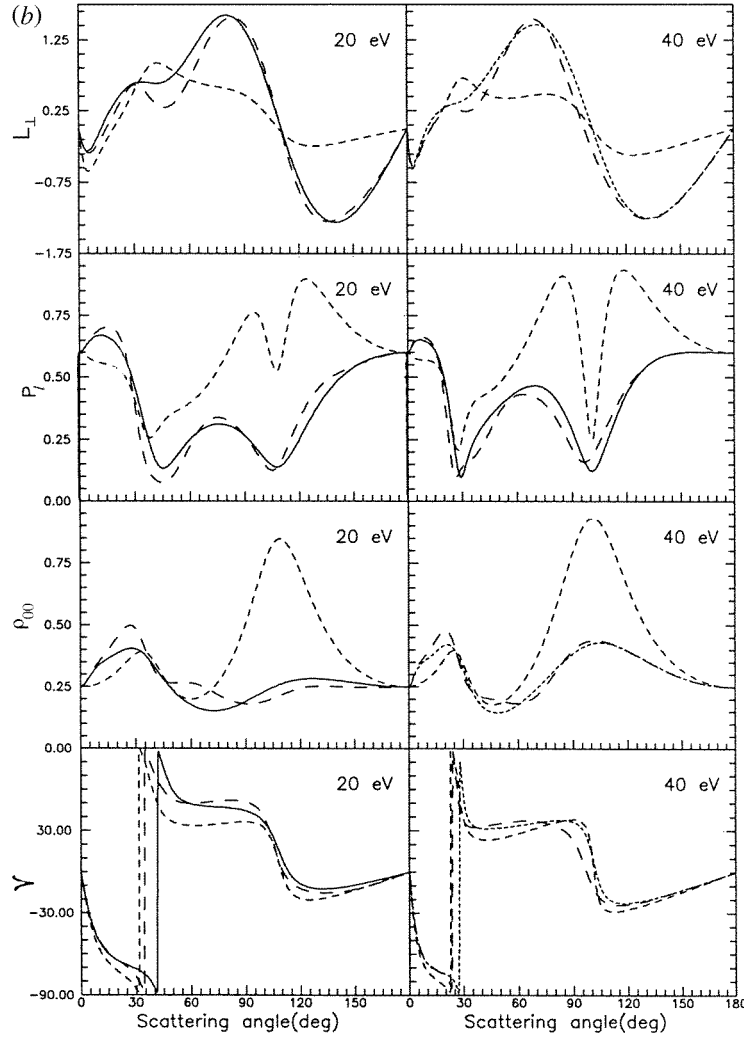$$I^z = \tfrac{2}{3}[\tfrac{69}{50} - \tfrac{19}{25}|a'_0|^2] \tag{26a}$$

(b)

Figure 6. (Continued)

and

$$I^y = \tfrac{1}{50}[\tfrac{81}{3} + \tfrac{38}{3}|a'_0|^2 - 19(\tfrac{2}{3})^{1/2}(\text{Re}(a'_0 a'^*_2) + \text{Re}(a'_0 a'^*_{-2}))]. \tag{26b}$$

Similar relations (equations (25) and (26)) can also be written for the spin-averaged case simply by replacing $(a'_m a'^*_{m'})$ by $\langle a'_m a'^*_{m'}\rangle$, where $\langle\rangle$ denotes spin averaging, i.e.

$$\langle a'_m a'^*_{m'}\rangle = [\tfrac{1}{4}a'^s_m a'^{s*}_{m'} + \tfrac{3}{4}a'^t_m a'^{t*}_{m'}]. \tag{27}$$

After taking into account the effect of the electron spin depolarization of the emitted light which reduces the Stokes parameters P_1-P_4, the reduced Stokes parameters $\bar{P}_1$ to $\bar{P}_4$ may be expressed in terms of the usual Stokes parameters by the following relations (Andersen *et al* 1988)

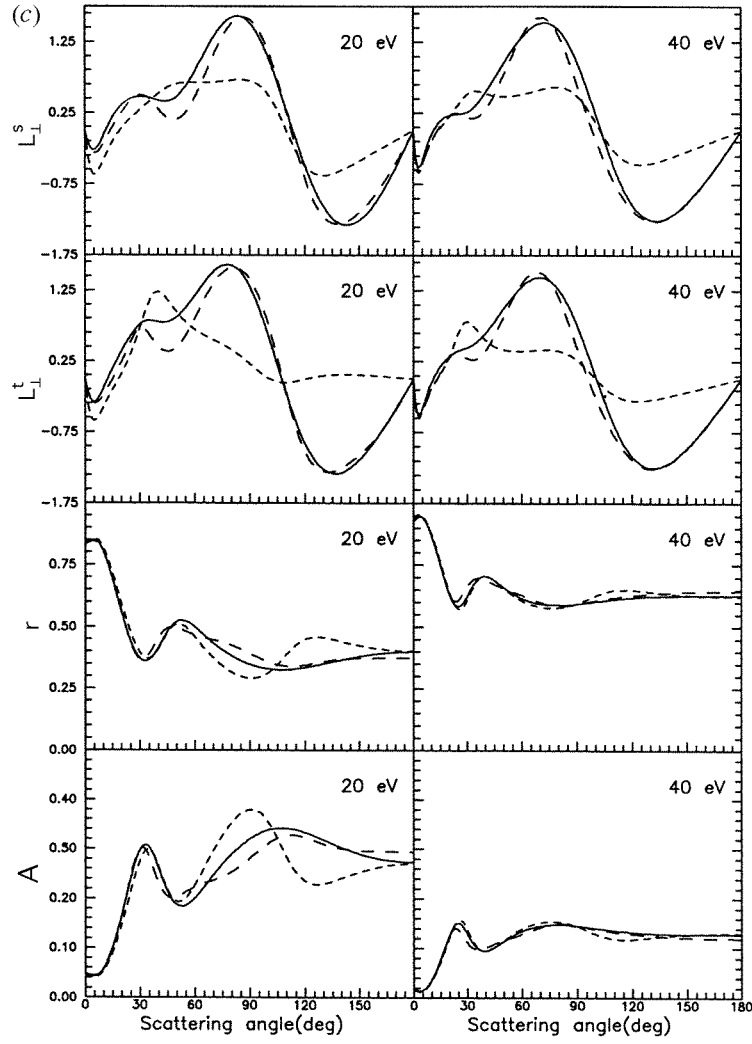$$\bar{P}_i = P_i \frac{I^z}{\tfrac{2}{3}(G_2 - 1) + I^z} \qquad (i = 1, 2) \tag{28a}$$

Figure 6. (Continued)

$$\bar{P}_3 = \left(\frac{G_2}{G_1}\right) P_3 \frac{I^z}{\frac{2}{3}(G_2 - 1) + I^z} \tag{28b}$$

$$\bar{P}_4 = P_4 \frac{2 - I^z(1 - P_1)}{\frac{2}{3}(2G_2 + 1) - I^z(1 - P_1)} \tag{28c}$$

where

$$I^z = \frac{2(1 + P_4)}{4 - (1 - P_1)(1 - P_4)} \qquad G_1 = \frac{23}{25} \qquad \text{and} \qquad G_2 = \frac{19}{25}. \tag{28d}$$

Here G_1 and G_2 are the depolarization factor coefficients.

Also the alignment and orientation parameters defined by Andersen *et al* (1988), i.e. the alignment angle, γ, linear polarization, P_l, height of electron charge cloud, ρ_{00}, and the angular momentum transferred perpendicular to the scattering plane, $L_\perp$, can be expressed
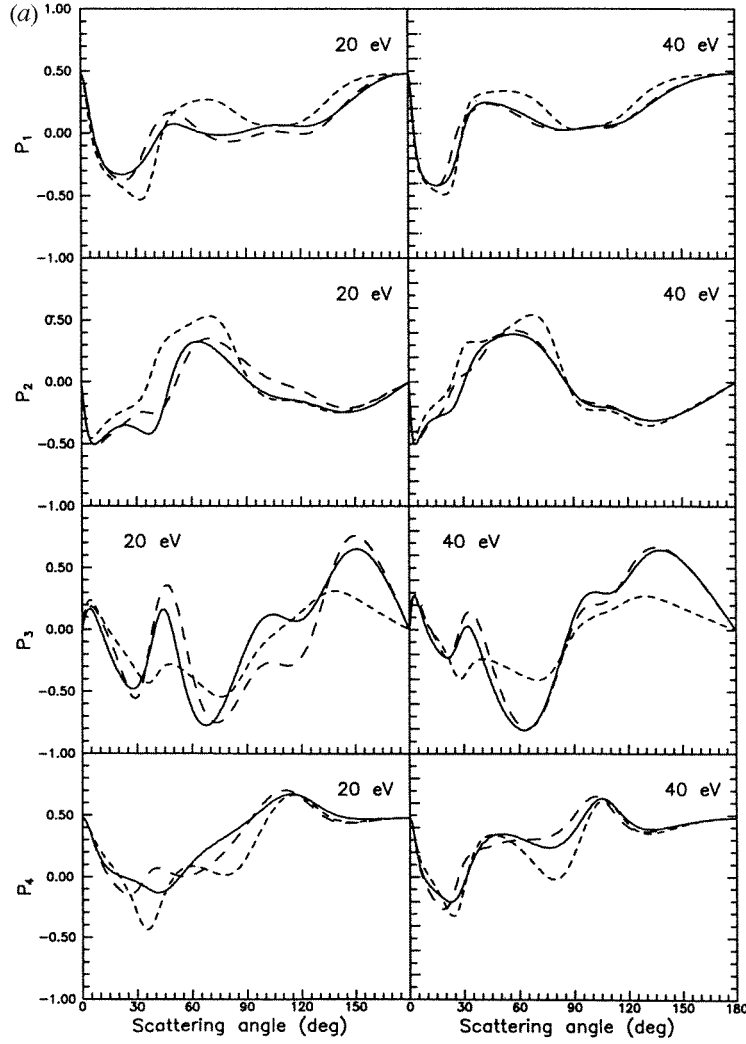
Figure 7. (*a*) Same as figure 6(*a*) but for the 3^2S–3^2D excitation in Na. (*b*) Same as figure 6(*b*) but for the 3^2S–3^2D excitation in Na. (*c*) Same as figure 6(*c*) but for the 3^2S–3^2D excitation in Na.

in terms of the reduced Stokes parameters as well as usual Stokes parameters by

$$\gamma = \tfrac{1}{2}\arg(\bar{P}_1 + \mathrm{i}\bar{P}_2) = \tfrac{1}{2}\arg(P_1 + \mathrm{i}P_2) \tag{29a}$$

$$P_l = \overline{|\bar{P}_1^2 + \bar{P}_2^2} \tag{29b}$$

$$L_\perp = -2\bar{P}_3\bar{I}^z = -\frac{2}{G_1}P_3 I^z \tag{29c}$$

$$\rho_{00} = \tfrac{2}{3}(1 - \bar{I}^z) = \tfrac{1}{2} + \frac{1}{G_2}(1 - \tfrac{3}{2}I^z) \tag{29d}$$

where

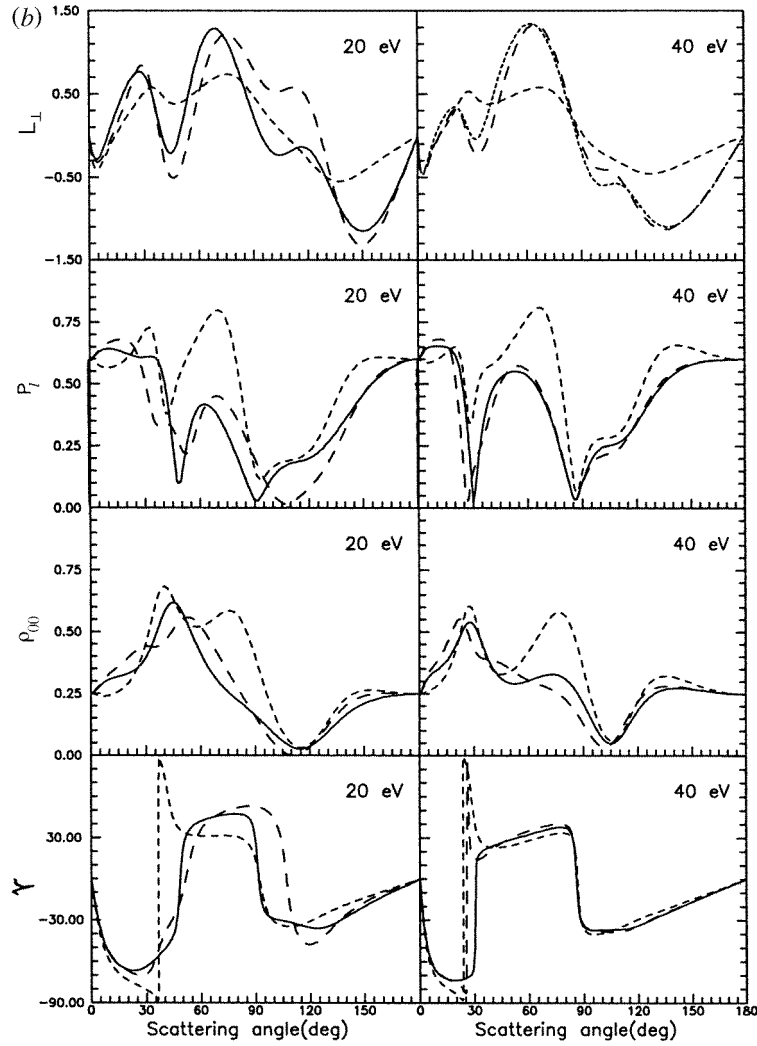$$G_2\bar{I}^z = \tfrac{2}{3}(G_2 - 1) + I^z. \tag{29e}$$

Figure 7. (Continued)

Again the spin-averaged orientation parameter $L_\perp$ is related to the spin-resolved orientation parameters $L_\perp^s$ and $L_\perp^t$ in the singlet and triplet modes by

$$L_\perp = \frac{L_\perp^s + 3r L_\perp^t}{(3r + 1)} \tag{30}$$

where r is the ratio of the triplet (σ^t) and singlet (σ^s) scattering cross sections, i.e.

$$r = \sigma^t / \sigma^s. \tag{31}$$

Finally, the spin asymmetry parameter is defined in terms of r as

$$A = \frac{(1 - r)}{(1 + 3r)} \tag{32}$$

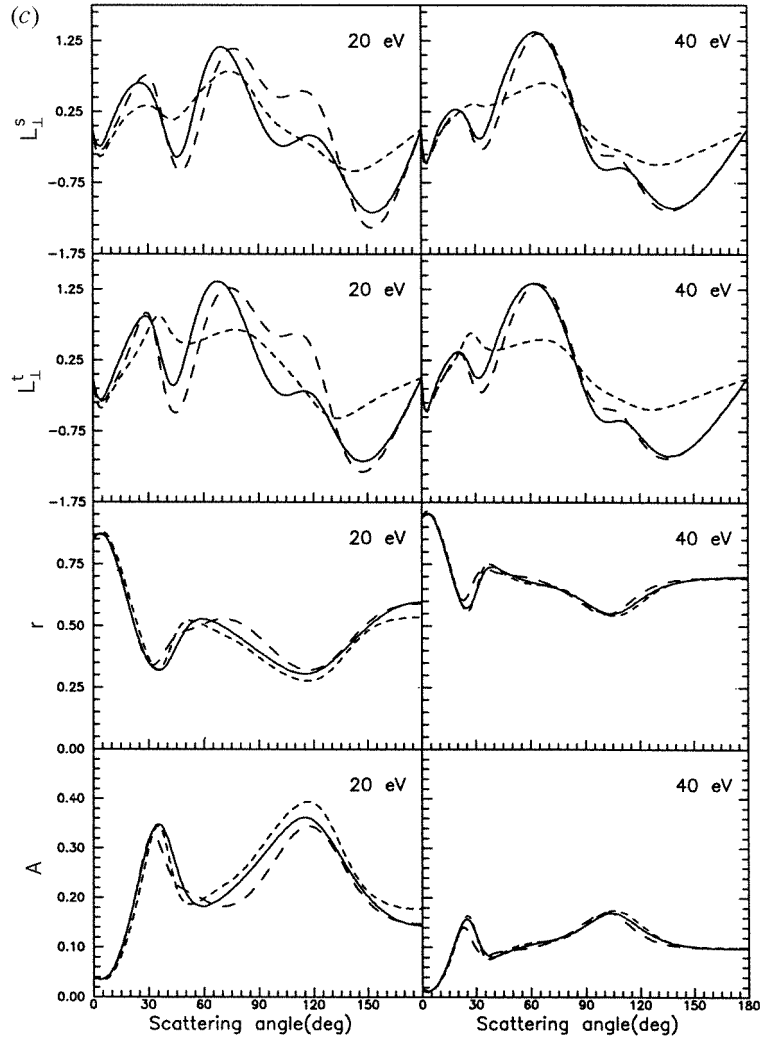for the scattering of spin-polarized electrons from spin-polarized alkali atoms.

(c)

Figure 7. (Continued)

To obtain different parameters (equations (25)–(32)) as defined earlier in terms of the singlet (triplet) scattering amplitudes $a_m'^{s(t)}$ in the natural coordinate frame, the following relations are used which connect the singlet (triplet) scattering amplitudes $a_m^{s(t)}$ in the collision reference frame which we essentially calculated using the DWA theory as described in section 2.1

$$a_2'^{s(t)} = (\tfrac{3}{8})^{1/2} a_0^{s(t)} + i a_1^{s(t)} - \tfrac{1}{2} a_2^{s(t)} \qquad (33a)$$

$$a_1'^{s(t)} = 0 \qquad (33b)$$

$$a_0'^{s(t)} = -\tfrac{1}{2} a_0^{s(t)} - (\tfrac{3}{2})^{1/2} a_2^{s(t)} \qquad (33c)$$

$$a_{-1}'^{s(t)} = 0 \qquad (33d)$$

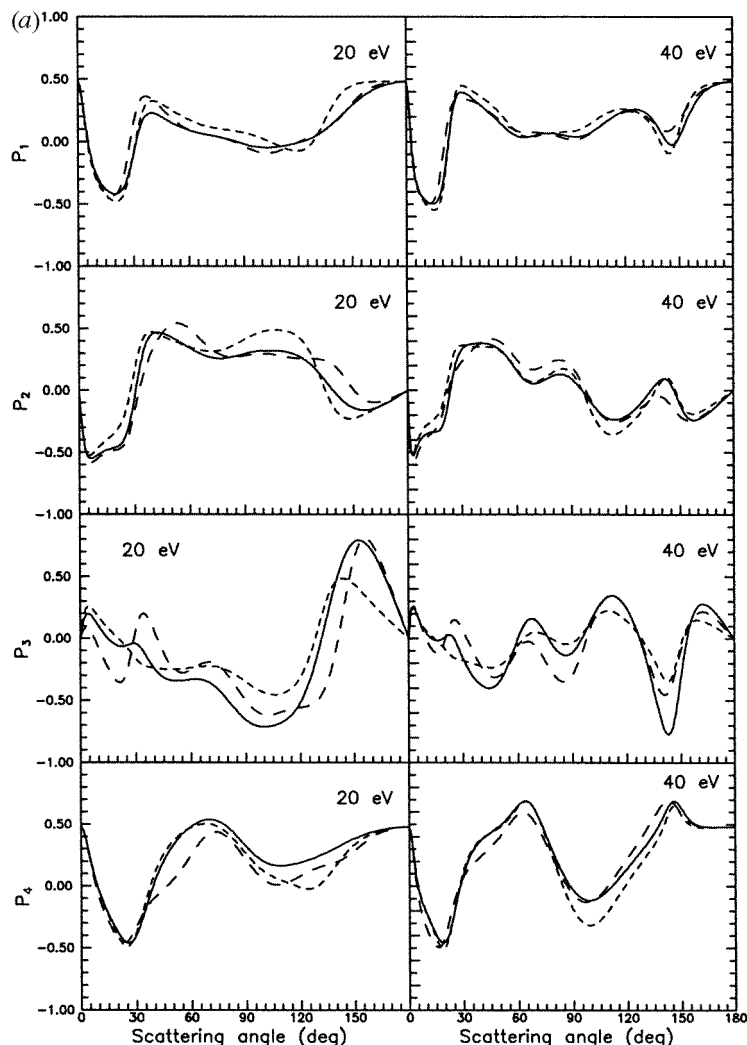$$a_{-2}'^{s(t)} = (\tfrac{3}{8})^{1/2} a_0^{s(t)} - i a_1^{s(t)} - \tfrac{1}{2} a_2^{s(t)}. \qquad (33e)$$

Figure 8. (*a*) Same as figure 6(*a*) but for the 4^2S–3^2D excitation in K. (*b*) Same as figure 6(*b*) but for the 4^2S–3^2D excitation in K. (*c*) Same as figure 6(*c*) but for the 4^2S–3^2D excitation in K.

3. Results and discussions

Using the DWA method described in the previous section, the results for the differential cross section (DCS), integrated cross section (TCS), Stokes parameters P_1, P_2, P_3 and P_4 and coherence parameters ($L_\perp$, P_l, γ and ρ_{00}) are obtained for n^2S–3^2D excitation in lithium ($n = 2$), sodium ($n = 3$) and potassium ($n = 4$) alkali atoms for the incident electron energy range of 10–100 eV. The calculations are carried out in all three versions of the DWA, i.e. the FF, IF and IIP models. Since there are no other previous calculations except for TCS for any of the Li, Na and K alkalis, we also carry out calculation in the first Born approximation (FBA) to compare with our various distorted-wave results. For this calculation we employ the same wavefunction as we use for our DWA calculations, so that a meaningful comparison can be made. Our FBA results for TCS agree very well with those
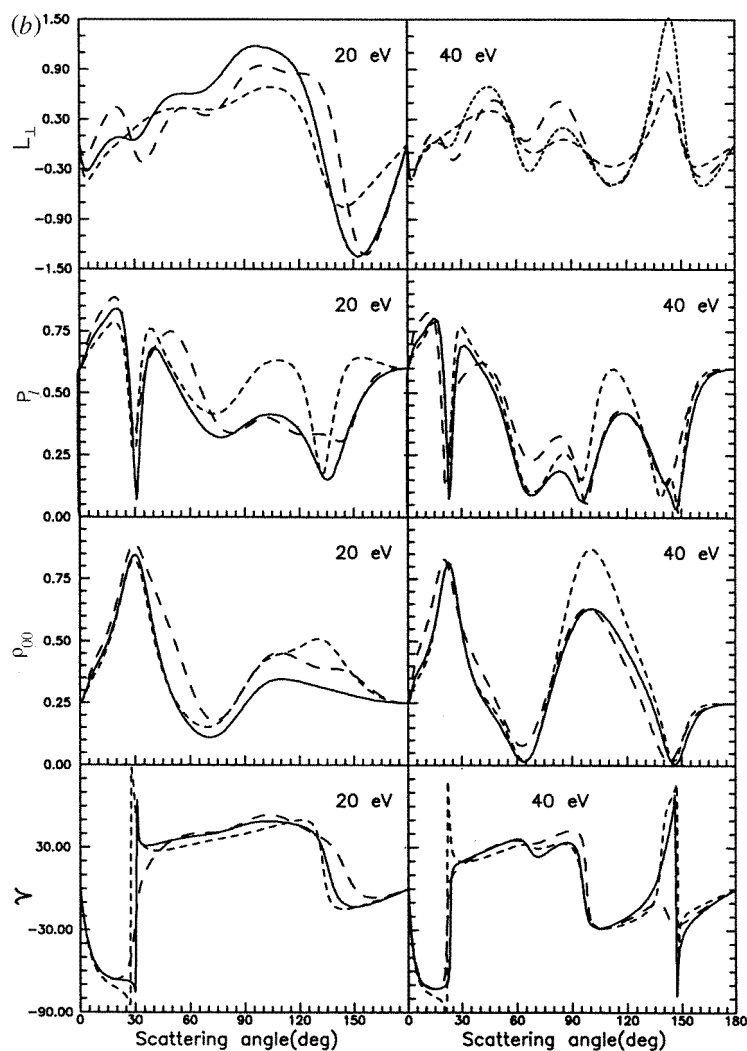
Figure 8. (Continued)

of Moiseiwitsch and Smith (1968) for Li (2^2S–3^2D), Na (3^2S–3^2D) and K (4^2S–3^2D) thus providing a check to our calculations.

In figure 1 we present our DWA results for TCS Q_T and Q_T^{90} obtained in our various models in the energy range of 10–100 eV for Li, Na and K. In addition, we also display our FBA results. For Q_T in figure 1(*a*) the comparison is made with the four-state close-coupling (4CC) results of Msezane (1988) for sodium and the unitarized Born approximation (UBA), unitarized distorted wave Born approximation (UDWBA) results of Mitroy (1993) and the seven-state close-coupling (7CC) results of Msezane *et al* (1992) for potassium. It can be seen from these figures that, as expected, the different theoretical results differ at lower energies where various effects, namely exchange, distortion and polarization, can contribute. Thereafter all the results tend to merge with increasing projectile energy. Further, in figure 1(*b*) and through tables 1–3, the results for Q_T^{90}, the total cross section measured at 90° to the incident electron beam direction, are shown. These include for comparison the
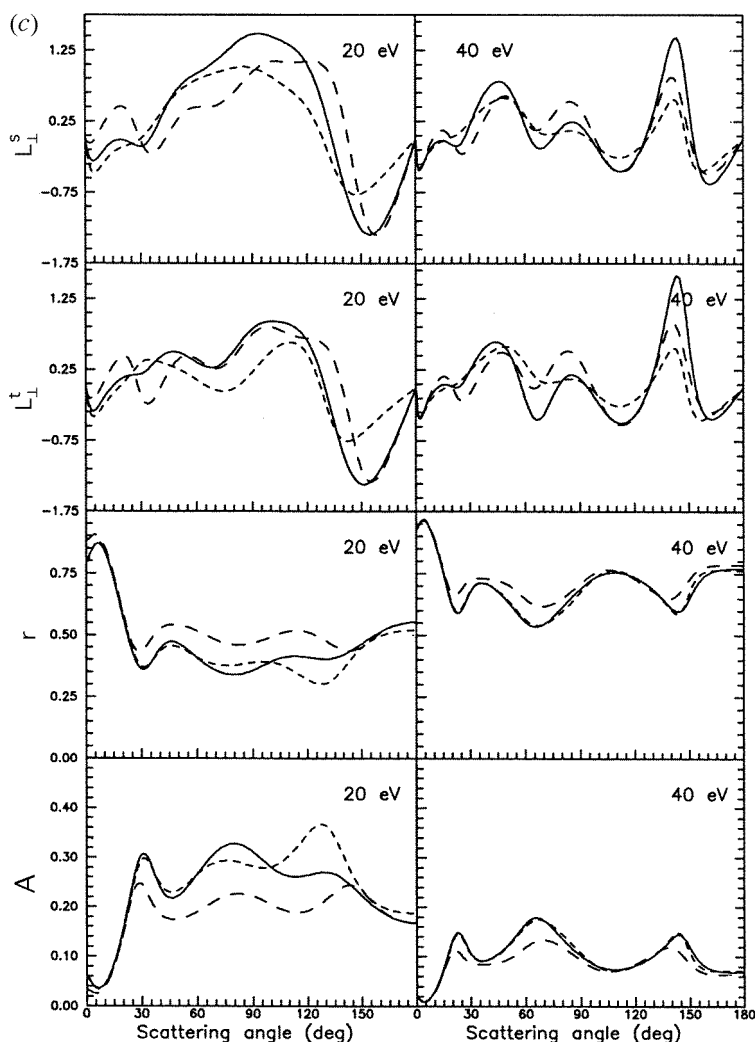
Figure 8. (Continued)

experimental data of Zajonc and Gallagher (1979) for Li and of Stumpf and Gallagher (1985) for Na. We have calculated the Q_T^{90} results in the DWA and the FBA using equations (21) and (23). The features observed here are similar to those seen in figure 1(a) for TCS Q_T i.e. the DWA results differ from the experimental data and FBA results for lower energies and then tend to merge at higher energies.

In figures 2–5, we have presented the differential cross section results for 3^2D excitation in Li, Na and K at selected energies where the DWA results can be considered reliable. First of all, in figure 2(a), (b) we compare the DCS results for Na at 10 and 54.4 eV, for which only the recent experimental data of Marinkovic′ *et al* (1992) exist. We compare these with our different DWA calculations. Since the data of Marinkovic′ *et al* (1992) are relative measurements, we normalize these as best fits to the large angle data with our DWA results in the FF model. The same normalization procedure for normalizing similar data for cadmium from Marinkovic′ *et al* (1991) was also adopted by Madison *et al* (1991).

However, a detailed discussion of the normalization of the experimental data of Marinkovic′ *et al* (1992) for elastic and inelastic 3^2S–3^2P excitation in Na has been given by Madison *et al* (1992). From the figure we see that though the DWA successfully reproduces the features observed in the experimental data, the data lie much above in the range of near forward scattering angles. Further, we also find that our results obtained using different models of the DWA differ from each other at larger scattering angles at the lower energy of 10 eV.

In figures 3–5, we present the DCS at incident electron energies of 20, 40 and 60 eV respectively, for Li, Na and K. In addition to our DWA results, in these figures we also report separately the FBA results. We find the FBA results are in agreement with the DWA results only at smaller angles and then they fall off rapidly with increasing scattering angle. This is a well known feature as discussed by Walters (1984), due to the dropping of the electron–nucleus interaction terms from the FBA T-matrix due to orthogonality of the target wavefunctions and due to the fact that we have not included the exchange contribution in the FBA T-matrix. Also the sharp minima present in the FBA are absent in all the DWA results. This feature is because of the difference in the projectile wavefunction in the two approximations (see Verma *et al* 1995). In fact, the FBA is essentially the DWA with zero distortion potential. In addition, on comparing the DWA results for Li, Na and K atoms at different energies we find that the structures present in DCS become more pronounced as the atomic number of the alkali atom increases, i.e. going from Li to K. In addition, the overall magnitudes of the DCS also increase as one moves from lithium to sodium to potassium. As expected, with the increase in energy the differences in the results obtained using our different models of the DWA decrease.

In figures 6–8 we present our other DWA results for excitation in lithium, sodium and potassium, respectively. In these figures we display the Stokes parameters P_ℓ–P_4 in (*a*); coherence parameters, namely alignment angle γ, linear polarization P_ℓ, angular momentum transferred perpendicular to the scattering plane $L_\perp$ and height of the charge cloud ρ_{00} are shown in (*b*); and finally in (*c*) the spin-resolved $L_\perp^s$, $L_\perp^t$, spin asymmetry and r are shown. These results are presented at electron impact energies of 20 and 40 eV. Unfortunately there are no other calculations reported so far for all these parameters for comparison. We have also carried out FBA calculations for these parameters, but for sake of clarity these are not shown. Also, as seen for P excitation in different atoms, the FBA calculations do not show any real structures and thus are not reliable (Andersen *et al* 1988). We see from the figures that in our DWA calculations the features present in Stokes parameters P_1–P_4 and coherence parameters γ, P_l, $L_\perp$ and ρ_{00} shift towards smaller angular region with increasing energy. We also see the structures differ with respect to the models and with different atoms. Since the parameters provide a sensitive testing of a theoretical model, other theoretical results and experiments would be desirable.

4. Conclusions

A complete study using the distorted-wave approximation theory has been carried out for the electron impact 3^2D excitation of the lighter alkali atoms from their ground states. Results for the total cross sections Q_T and Q_T^{90} are presented and compared with other available data in the energy range 10–100 eV. Further, the differential cross section results at various energies for Li(2^2S–3^2S), Na(3^2S–3^2D) and K(4^2S–3^2D) are reported. Finally, for the first time results are presented for Stokes parameters P_1–P_4, coherence parameters γ, P_l, $L_\perp$ and ρ_{00} and the spin-resolved $L_\perp^s$, $L_\perp^t$, spin asymmetry A and r. We hope that our present work will initiate more theoretical and experimental studies so that a meaningful conclusion can be drawn.

Acknowledgments

References

Andersen N, Gallagher J W and Hertel I V 1988 *Phys. Rep.* **165** 1
Becker K, Crow A and McConkey J W 1992 *J. Phys. B: At. Mol. Opt. Phys.* **25** 3885
Bray I, Fursa D V and McCarthy I E 1995 *Phys. Rev.* A **51** 500
Crowe A, Donnelly B P, McLaughlin D T, Bray I and Fursa D V 1994 *J. Phys. B: At. Mol. Opt. Phys.* **27** L795
Daniele R 1979 *J. Chem. Phys.* **70** 3462
——1980 *J. Chem. Phys.* **72** 1276
Farrell D F, Chwirot S, Srivastava R and Slevin J 1990 *J. Phys. B: At. Mol. Opt. Phys.* **23** 315
Furness J B and McCarthy I E 1973 *J. Phys. B: At. Mol. Phys.* **6** 2280
Itikawa Y 1986 *Phys. Rep.* **143** 69
Jhanwar B L and Khare S P 1976 *J. Phys. B: At. Mol. Phys.* **9** L527
Katiyar A K and Srivastava R 1987 *J. Phys. B: At. Mol. Phys.* **20** L821
——1989 *Phys. Rev.* A **40** 1289
Madison D H, Bartschat K and McEachran R P 1992 *J. Phys. B: At. Mol. Opt. Phys.* **25** 5199
Madison D H, Bartschat K and Srivastava R 1991 *J. Phys. B: At. Mol. Opt. Phys.* **24** 1839
Marinkovic' B, Pejčev V, Filipovic' D, Čadez I and Vuškovic' L 1992 *J. Phys. B: At. Mol. Opt. Phys.* **25** 5179
Marinkovic' B, Pejčev V, Filipovic' D and Vuškovic' L 1991 *J. Phys. B: At. Mol. Opt. Phys.* **24** 1817
Mikosza A G, Hippler R, Wang J B and Williams J F 1994 *Z. Phys.* D **30** 129
Miller T M and Bederson B 1977 *Adv. At. Mol. Phys.* **13** 1
Mitroy J 1993 *J. Phys. B: At. Mol. Opt. Phys.* **26** 2201
Mittleman M H and Watson K M 1960 *Ann. Phys., NY* **10** 268
Moiseiwitsch B L and Smith S J 1968 *Rev. Mod. Phys.* **40** 238
Mott N F and Massey H S W 1965 *The Theory of Atomic Collisions* (London: Oxford University Press)
Msezane A Z 1988 *Phys. Rev.* A **37** 1787
Msezane A Z, Awuah P, Hiamang S and Allotey F K A 1992 *Phys. Rev.* A **46** 6949
Percival I C and Seaton M J 1958 *Phil. Trans. R. Soc.* A **251** 113
Slevin J A and Chwirot S 1990 *J. Phys. B: At. Mol. Opt. Phys.* **23** 165
Stumpf B and Gallagher A 1985 *Phys. Rev.* A **32** 3344
Szasz L and McGinn G 1967 *J. Chem. Phys.* **47** 3495
Verma S and Srivastava R 1994 *Phys. Rev.* A **50** 2269
——1995a *Can. J. Phys.* in press
——1995b *J. Phys. B: At. Mol. Opt. Phys.* **28** 4823
——1996 *J. Phys. B: At. Mol. Opt. Phys.* **29** in press
Verma S, Srivastava R and Itikawa Y 1995 *J. Phys. B: At. Mol. Opt. Phys.* **28** 1023
Vučic' S, Potvliege R M and Joachain C J 1987 *J. Phys. B: At. Mol. Phys.* **20** 3157
Walters H R J 1984 *Phys. Rep.* **116** 1
Williams J F and Wang J B 1994 *Adv. At. Mol. Opt. Phys.* **32** 407
Zajonc A and Gallagher A 1979 *Phys. Rev.* A **20** 1393