

The scattering of electrons by sodium atoms

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MS received 23 March 1972

Abstract. Four state exchange ($3s-3p-4s-3d$) close coupling equations are solved for the scattering of electrons by sodium atoms at incident energies up to 5 eV. The results are presented in such a form that a number of different measurable quantities may be readily extracted from tables and simple formulae. Total and differential (elastic and inelastic) cross sections, and the polarization of the resonance doublet radiation, are calculated. Results obtained do not differ to any great extent from two state ($3s-3p$) calculations of the same quantities. Comparison with available experimental data is made; the total cross section disagrees with the experiment of Brode; and the results obtained for the polarization of the radiation fail to remove the discrepancy between the experiment of Hafner and Kleinpoppen and the two state calculations by Karule. The polarization agrees well with more recent experimental results, as do the differential elastic scattering and $3s \rightarrow 3p$ excitation cross sections.

1. Introduction

The low energy scattering of electrons by alkali metal atoms has been the subject of much recent work and discussion. In the case of elastic scattering, detailed reviews of the theoretical and experimental data have been given by Bederson (1970a). A discussion of experimental data for total scattering is contained in the review by Bederson and Kieffer (1971). Evidence is now accumulating that the absolute experimental results of Brode (1929) are in all cases too large by about a factor of two in magnitude, and also in error in the energy variation.

For scattering by alkalis at low energies, a two state (n_0s-n_0p) exchange close coupling calculation (n_0s being the ground state) ought to be adequate, taking account as it does of almost all of the (large) dipole polarizability of the atom, which plays a major role in the low energy scattering. However, the close coupling calculations by Karule (1965) and by Karule and Peterkop (1965) are smaller by about a factor of two than Brode's results for the lighter alkalis, that is, lithium, sodium and potassium, as are the calculations by Burke and Taylor (1969) for lithium and by Salmona (1965) for sodium. Relative measurements of the total cross section by Perel *et al* (1962) for lithium and sodium, which are normalized using Brode's potassium result, also show somewhat different structure at low energies. Absolute experiments by Collins *et al* (1971) for

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‡ Operated jointly by the University of Colorado and the National Bureau of Standards.

potassium, however, give results in good agreement with Karule (1965) and Karule and Peterkop for differential and differential-exchange as well as total cross sections. The spin-exchange cross section has also been measured by Campbell *et al* (1971). Absolute total cross sections for potassium, rubidium and cesium measured by Visconti *et al* (1971) are also in substantial disagreement with Brode (again by about a factor of two), but agree well with Karule (1965), Karule and Peterkop, and Collins *et al* for potassium. For cesium the results of Visconti *et al* are significantly lower than the Karule (1965) results in the elastic scattering region, but agree well with the results of Karule and Peterkop at higher energies.

Experimental studies of electron-atom collisions which involve the use of various combinations of polarized electron and atom beams, with spin analysis of the scattered electrons or atoms, or observation of the intensity and polarization of the emitted line intensity following excitation, have been discussed in general terms by Bederson (1969, 1970b) and Kleinpoppen (1971). Suitable experimental arrangements can yield information on the direct (Hils *et al* 1972) and exchange (Collins *et al* 1971) scattering amplitudes, or their relative phase, for elastic or total scattering, or for excitation of different magnetic substates (Goldstein *et al* 1972). Such experiments obviously provide a much more sensitive test of theory than do measurements of the total or total-differential scattering cross sections, calculation of which involves more integration and summation, thereby smoothing out inaccuracies.

Measurements for potassium of absolute differential (Slevin *et al* 1972) and relative differential (Gehenn and Wilmers 1971, and Hils *et al* 1972) and differential-direct (Hils *et al*) cross sections for elastic scattering, absolute differential (Slevin *et al*) and the ratio of differential atomic spin-exchange to total differential cross sections in excitation (Rubin *et al* 1969, and Goldstein *et al* 1972), are all in reasonable agreement with Karule (1965) and Karule and Peterkop. Relative measurements of differential cross sections for elastic scattering by sodium have also been performed (Andrick *et al* 1972, and Gehenn and Reichert 1972), and again are in good agreement with Karule (1965) and Karule and Peterkop.

When one considers inelastic scattering, a sensitive test of theory is provided by a calculation of the polarization of the line radiation emitted following excitation by electron impact. For sodium and lithium, Karule (1970) has calculated the polarization of the doublet resonance radiation from the theory given by Percival and Seaton (1958) and Flower and Seaton (1967), using the two state reactance matrices of Karule and Peterkop (1965). The results obtained lie somewhat below the experimental results of Hafner and Kleinpoppen (1967), the discrepancy being greater in the case of sodium. The lithium calculations agree quite well with those of Burke and Taylor (1969). Feautrier (1970), also for lithium, has shown that by using a close coupling method modified to take full account of the polarizability of the atomic states, agreement with experiment is improved. On the other hand, recent experiments by Enemark and Gallagher (1972) and Gould (1970) for sodium yielded results in good agreement with the Karule (1970) calculation.

For excitation of the 3p state of sodium, the experimental results of Haft (1933) and Christoph (1935) are in reasonable agreement with the unitarized Born approximation calculation by Salmona and Seaton (1961) at high energies (> 50 eV) and in fair agreement with the calculations by Karule and Peterkop (1965), and Salmona (1965) at low energies (the latter, however, use Hartree-Fock eigenenergies for the atom, resulting in a displacement of the threshold and making direct comparison difficult). The experimental results of Enemark and Gallagher (1972), normalized to the first Born approximation above 250 eV and corrected for cascade using the cross sections measured by Zapesochnyi

and Shimon (1965), are about half the results of Haft and of Christoph in the intermediate energy region, while being considerably larger than the measured results of Zapesochnyi (1967). Experimental results very similar to those of Enemark and Gallagher have also been obtained by Gould (1970), and both are in excellent agreement with the calculation by Karule and Peterkop. Two state and three state ($3s-3p-3d$) close coupling calculations without exchange in the intermediate energy range for sodium have been made by Barnes *et al* (1965) and Korff *et al* (1971), respectively, which fall between the experimental results of Haft and of Christoph, and those of Enemark and Gallagher and of Gould.

In earlier work by one of us (Norcross 1971) phase shifts for elastic scattering of electrons by lithium and sodium at energies below the first excitation threshold were obtained, using a two state close coupling approximation with a scaled Thomas-Fermi statistical model potential, modified by a term allowing for core polarization, to describe the target atom. The form chosen for the potential contains two parameters which may be adjusted so that the experimental energy eigenvalues are reproduced. This avoids the difficulties associated with the use of Hartree-Fock functions for the target atom, which give inaccurate energy eigenvalues, and which have been shown to lead to significant errors (Burke and Moores 1968). The computer code used in this and the present work is an adaptation of one originally supplied by Professor P G Burke.

The results obtained by Norcross (1971) are in good agreement with those of Burke and Taylor (1969), and of Karule (1965), except at thermal energies. In the case of sodium the calculated spin-flip cross section differed substantially from the Karule (1965) result,[†] and also from the measured values of Dehmelt (1958) and Balling (1966).

In the present work, we extend the elastic scattering results to higher energies, and investigate the effects, in the case of sodium, of including the $4s$ and $3d$ states in the close coupling expansion, in order to check upon its convergence for the case of elastic scattering and consequently the accuracy of the two state calculations; and for inelastic scattering both to improve upon previous calculations and to provide additional results for comparison with experiment. Of particular interest are the values of the $3s \rightarrow 4s$ and $3s \rightarrow 3d$ excitation cross sections near threshold.

Once the scattering problem has been solved and reactance (or scattering) matrices obtained, a potential wealth of information is available; and the multitude of scattering parameters set out by Kleinpoppen (1971) and others may be computed with relatively little effort. Since space considerations do not permit tabulation of more than a small amount of the total material, some thought was given to the form in which the present results should be presented. It was decided therefore that the most useful quantities to tabulate in addition to total cross sections are the squares of all the direct, exchange and interference amplitudes for elastic and inelastic scattering, together with the direct, exchange and interference partial cross sections for excitation of the $3p$ magnetic sub-states. These are the basic parameters by means of which all of the measurable quantities may be obtained, using simple formulae. A general computer program has been developed by one of us (Moores 1971) to extract any of this information from the reactance matrices.

2. Theory

The system of coupled integro-differential equations describing the scattering of electrons by alkali-like systems has been derived elsewhere (eg, Salmona and Seaton 1961) and will not be given here. In the present case, of course, all terms involving core electrons

[†] Footnote added in proof. Dr Karule has informed us that results of revised calculations are in much agreement.

disappear and the equations are similar in form to those for electron-hydrogen scattering (Percival and Seaton 1957). Solution of these equations with the appropriate boundary conditions yields the reactance matrix, \mathbf{R} , and hence the \mathbf{T} matrix:

$$\mathbf{T} = -2i\mathbf{R}(1 - i\mathbf{R})^{-1} \quad (2.1)$$

from which all measurable quantities may be computed.

2.1. Total cross sections

The total elastic scattering cross section in atomic units (a_0^2) is given by

$$Q = \frac{\pi}{4k_i^2} \sum_{L,S} (2L+1)(2S+1) |T_{11}^{S,L}|^2 \quad (2.2)$$

where L and S are the total angular momentum and spin of the system, and k_i^2 is the incident electron energy in rydbergs. The spin-flip cross section is given by

$$Q_{\text{sf}} = \frac{\pi}{4k_i^2} \sum_L (2L+1) |T_{11}^{1,L} - T_{11}^{0,L}|^2. \quad (2.3)$$

For inelastic scattering, we have

$$Q(3s \rightarrow 3p) = \frac{\pi}{4k_i^2} \sum_{L,S,l_2} (2L+1)(2S+1) |T_{3sL,3pl_2}^{S,L}|^2 \quad (2.4)$$

and the corresponding spin-flip cross section

$$Q_{\text{sf}}(3s \rightarrow 3p) = \frac{\pi}{4k_i^2} \sum_{L,l_2} (2L+1) |T_{3sL,3pl_2}^{1,L} - T_{3sL,3pl_2}^{0,L}|^2. \quad (2.5)$$

The total cross section for excitation of the state with magnetic quantum number M is given by

$$Q_M(3s \rightarrow 3p) = \frac{\pi}{4k_i^2} \sum_{S,l_2} (2S+1) \left| \sum_L (2L+1)^{1/2} i^{L-l_2} C_{M-M_0}^{1,l_2,L} T_{3sL,3pl_2}^{S,L} \right|^2. \quad (2.6)$$

2.2. Differential scattering and spin polarization

2.2.1. Elastic scattering. The theory of differential scattering and spin polarization in elastic scattering by one electron atoms has been developed by Burke and Schey (1962) and summarized by Burke and Taylor (1969). The scattering amplitudes $f^\pm(\theta)$ are defined by

$$f^\pm(\theta) = \frac{i}{2k_i} \sum_{L=0}^{\infty} (2L+1) P_L(\cos \theta) T_{11}^{S,L} \quad (2.7)$$

where the total spin $S = 0$ for the singlet (+) and $S = 1$ for the triplet (−) cases. These amplitudes are related to the direct amplitude $f(\theta)$ and the exchange amplitude $g(\theta)$ by

$$f^\pm(\theta) = f(\theta) \pm g(\theta). \quad (2.8)$$

Expressions are then obtained for the differential cross section and the spin polarization

of atoms and electrons after scattering, given the spin polarizations and the spin correlation tensor before scattering, in terms of the five functions

$$\begin{aligned}
 k(\theta) &= \frac{3}{4}|f^-(\theta)|^2 + \frac{1}{4}|f^+(\theta)|^2 \\
 &= \frac{1}{2}|f|^2 + \frac{1}{2}|g|^2 + \frac{1}{2}|f-g|^2 \\
 n(\theta) &= k(\theta) - |g|^2 \\
 p(\theta) &= k(\theta) - |f|^2 \\
 m(\theta) &= k(\theta) - |f|^2 - |g|^2 = n(\theta) + p(\theta) - k(\theta) \\
 q(\theta) &= \frac{1}{2} \operatorname{Im}\{(f-g)(f+g)^*\}.
 \end{aligned} \tag{2.9}$$

For a scattering experiment with either the electrons or atoms having random spins initially, the differential cross section $\sigma(\theta)$ is equal to $k(\theta)$; $p(\theta)/k(\theta)$ is the polarization of an initially unpolarized electron beam after scattering by a fully polarized atom beam, whose final polarization is then $n(\theta)/k(\theta)$; and $n(\theta)/k(\theta)$ is the final polarization of a fully polarized electron beam after scattering by an unpolarized atom beam, whose final polarization is $p(\theta)/k(\theta)$. The general case of both beams initially polarized along different axes is rather complex, requiring knowledge of the initial spin correlation and the parameter $q(\theta)$; but a special case of this, both beams polarized along the same axis, has been discussed by Kleinpopp (1971), which involves only $m(\theta)$ in addition to $k(\theta)$, $n(\theta)$ and $p(\theta)$.

The differential spin-flip cross section is defined by

$$\sigma_{\text{SF}}(\theta) = \frac{1}{4}|f^- - f^+|^2 = |g|^2. \tag{2.10}$$

This quantity is often incorrectly referred to as the spin-exchange cross section, which is defined by

$$\sigma_{\text{SE}}(\theta) = \frac{1}{2}|g|^2. \tag{2.11}$$

It follows that determination of the moduli of the scattering amplitudes and the magnitude of the phase difference between them can be accomplished either by independent measurements of the singlet, triplet and spin-flip cross sections; or, in terms of the quantities in (2.9), of the direct, exchange and interference cross sections. The sign of the phase difference can only be determined by an additional experiment involving spin correlation, that is, measurement of $q(\theta)$.

2.2.2. Excitation of the 3p-state. In this case we have three separate scattering amplitudes for each total spin state, corresponding to excitation of the states $M = +1, 0, -1$, with final electron energy k_f^2 , given by

$$f_M^\pm(\theta, \phi) = \frac{1}{2i} \left(\frac{4\pi}{k_i k_f} \right)^{1/2} \sum_{L, l_2 = L \pm 1} i^{L-l_2} (2L+1)^{1/2} C_{LM0}^{l_2} Y_{l_2}^{-M}(\theta, \phi) T_{3sL, 3pl_2}^{S, L}. \tag{2.12}$$

For $|M| = 1$ we have $f_{\pm 1}^\pm = (f_{\pm 1}^\pm)^*$. We may also define direct and exchange amplitudes $f_M(\theta, \phi)$ and $g_M(\theta, \phi)$ by equations analogous to (2.8). Let us also define the quantities

$$k_M(\theta) = \frac{3}{4}|f_M^-|^2 + \frac{1}{4}|f_M^+|^2 = \frac{1}{2}|f_M|^2 + \frac{1}{2}|g_M|^2 + \frac{1}{2}|f_M - g_M|^2 \tag{2.13}$$

and

$$k(\theta) = \sum_M k_M(\theta) = k_0(\theta) + 2k_1(\theta). \tag{2.14}$$

For unorientated atoms and/or electrons the differential cross section for excitation of state M is given by

$$\sigma_M(\theta) = \frac{k_f}{k_i} k_M(\theta) \quad (2.15)$$

and the total differential cross section is

$$\sigma(\theta) = \sum_M \sigma_M(\theta) = \sigma_0(\theta) + 2\sigma_1(\theta). \quad (2.16)$$

The differential spin-flip cross section for the electrons is

$$\sigma_{\text{SF}}(\theta) = \frac{k_f}{k_i} (|g_0|^2 + 2|g_1|^2). \quad (2.17)$$

Clearly integration of (2.15), (2.16) and (2.17) over solid angle leads directly to (2.6), (2.4) and (2.5).

As far as the theory of spin polarization is concerned, it is a simple extension of the theory of Burke and Schey (1962) if all spin-orbit effects are ignored. In a typical scattering experiment, at least for light atoms, the collision time is so small that spin-orbit effects during the collision may indeed be neglected, and hence the spin of the electrons is only affected by the exchange interaction with the atom.

One can also consider making observations of the atoms rather than electrons. It is not generally possible to make observations on excited atoms, since their radiative lifetimes are generally short compared with their time-of-flight in a typical experiment. If the radiative lifetime is, however, long compared with the characteristic time for spin-orbit relaxation, a further change of spin in the excited state may occur before observation can be made.

In recoil-type experiments, such as those of Rubin *et al* (1969) and Goldstein *et al* (1972) observation of change of spin of the atoms after excitation into the ^2P state and subsequent decay to the ^2S state is made. This process can be described as one in which the atoms are originally in state $^2\text{S}, M_S$, and finally in state $^2\text{S}, M'_S$, with the corresponding electron spins m_s and m'_s , and the electrons are scattered into the angles (θ, ϕ) . From the theory of Percival and Seaton (1958) the differential cross section, summed over the polarizations of the emitted photons is given by

$$\sigma_{M_S m_s, M'_S m'_s}(\theta, \phi) = \frac{C_v}{A} \frac{k_f}{k_i} \sum_{\mu} \left| \sum_{\substack{JM_J \\ MM'_S}} \langle ^2\text{S}, M'_J | T_{1\mu} | ^2\text{P}, JM_J \rangle C_{M'_S M'_J}^{1/2 \ 1 \ J} F(J) f_M(M_S m_s, M'_S m'_s | \theta \phi) \right|^2 \quad (2.18)$$

where A is the total probability for emission of a photon of frequency ν , $C_v = 64\pi^4 e^2 \nu^3 / 3hc^3$ and

$$f_M(M_S m_s, M'_S m'_s | \theta \phi) = \sum_{SM'_S} C_{M'_S m'_s}^{1/2 \ 1/2 \ S} f_M^S(\theta \phi) C_{M_S m_s}^{1/2 \ 1/2 \ S} \quad (2.19)$$

where $f_M^S(\theta, \phi)$ is given by (2.12) with $f_M^0 \equiv f_M^+$ and $f_M^1 \equiv f_M^-$.

The vectors $F(J)$ are defined by Percival and Seaton (1958) and depend on the ratio $\epsilon = 2\pi\delta\nu/A$ of the fine structure separation $\delta\nu = (1/h)\{E(^2\text{P}_{3/2}) - E(^2\text{P}_{1/2})\}$ to the transition probability A from the excited state. Hyperfine structure has been neglected (the experiments mentioned above take place in a magnetic field strong enough to

uncouple the electron and nuclear spins). For excitation of the fine structure levels of sodium, we have $\epsilon \gg 1$ and the vectors $F(1/2)$ and $F(3/2)$ are orthogonal, a fact which permits reduction of (2.18) to

$$\sigma_{M_S m_s, M_S' m_s'}(\theta) = \frac{k_f}{k_i} \sum_{\substack{\mu J M_J \\ M M_S}} (C_{M_S' - \mu M_J}^{1/2 \ 1 \ J} C_{M_S \ M M_J}^{1/2 \ 1 \ J})^2 |f_M(M_S m_s, M_S' m_s' | \theta \phi) \delta_{M_S' + m_s', M_S + m_s}|^2 \quad (2.20)$$

where the squared amplitude is one of either $|f_M|^2$, $|g_M|^2$ or $|f_M - g_M|^2$.

Given various combinations of initial electron and atom polarization, one may readily obtain from (2.20) expressions for the differential excitation cross sections and final electron and atom polarization. All of the quantities involved may thus be expressed in terms of the amplitudes $|f_M|^2$, $|g_M|^2$ and $|f_M - g_M|^2$.

For example, let us consider the simple cases of one of the initial electron or atom beams unpolarized, the other with polarization P_e or P_a . For $P_e = 0$, the final electron polarization is

$$P_e(\theta) = \frac{I(\uparrow) - I(\downarrow)}{I(\uparrow) + I(\downarrow)}$$

where $I(\uparrow) = I(m_s' = 1/2)$ and $I(\downarrow) = I(m_s' = -1/2)$, after summing $\sigma_{M_S m_s, M_S' m_s'}(\theta)$ over m_s and M_S' ; and the final atom polarization is

$$P_a(\theta) = \frac{I(\uparrow) - I(\downarrow)}{I(\uparrow) + I(\downarrow)}$$

where $I(\uparrow) = I(M_S' = 1/2)$ and $I(\downarrow) = I(M_S' = -1/2)$, after summing $\sigma_{M_S m_s, M_S' m_s'}(\theta)$ over m_s and m_s' . The resulting expressions are

$$k(\theta)P_e(\theta) = P_a\{k(\theta) - |f_0|^2 - 2|f_1|^2\} \quad (2.21)$$

and

$$k(\theta)P_a(\theta) = \frac{1}{9}P_a\{k_0 + 10k_1 - |g_0|^2 - 10|g_1|^2\}. \quad (2.22)$$

Analogous expressions for the case of $P_a = 0$ are

$$k(\theta)P_e(\theta) = P_e\{k(\theta) - |g_0|^2 - 2|g_1|^2\} \quad (2.23)$$

and

$$k(\theta)P_a(\theta) = \frac{1}{9}P_e\{k_0 + 10k_1 - |f_0|^2 - 10|f_1|^2\}. \quad (2.24)$$

Note that the quantities in brackets in (2.21) and (2.23) are, respectively, the same as the quantities $p(\theta)$ and $n(\theta)$ defined in (2.9), except for the sum over M . This is to be expected, since the spin-orbit effects do not affect the final electron polarization.

The experiments of Rubin *et al* (1969) and Goldstein *et al* (1972) treat a special case of (2.22), that is measurements of the fraction of scattered atoms excited from a beam with $P_a = 1$ which have decayed to the opposite spin state. This ratio $R(\theta)$ is simply

$$\begin{aligned} R(\theta) &= \frac{1}{2}(1 - P_a(\theta)) \\ &= (8k_0 + 8k_1 + |g_0|^2 + 10|g_1|^2)/18k(\theta). \end{aligned} \quad (2.25)$$

2.3. Polarization of the line radiation

Expressions for the intensity of the emitted line radiation with a given polarization, neglecting hyperfine structure, may be obtained by integrating each term in (2.20) of

the summation over μ , over solid angles of the ejected electron. All these formulae involve the integrated amplitudes

$$\begin{aligned} D_M &= \frac{k_f}{k_i} \int |f_M|^2 d\Omega \\ E_M &= \frac{k_f}{k_i} \int |g_M|^2 d\Omega \\ I_M &= \frac{k_f}{k_i} \int |f_M - g_M|^2 d\Omega. \end{aligned} \quad (2.26)$$

The total cross section for excitation of the state M is clearly just half the sum of D_M , E_M and I_M †.

For example, the circular polarization of the D_1 and D_2 lines of sodium following excitation of atoms with initial spin polarization P_a by unpolarized electrons is given by

$$P(D_1) = \frac{1}{P_a} \frac{I^{\sigma+} - I^{\sigma-}}{I^{\sigma+} + I^{\sigma-}} = \frac{\Delta_0 - 2\Delta_1}{Q_0 + 2Q_1} \quad (2.27)$$

and

$$P(D_2) = \frac{1}{P_a} \frac{I^{\sigma+} - I^{\sigma-}}{I^{\sigma+} + I^{\sigma-}} = \frac{\Delta_0 + 4\Delta_1}{Q_0 + 5Q_1} \quad (2.28)$$

where

$$\Delta_i = Q_i - E_i \quad (2.29)$$

$I^{\sigma\pm}$ are the relative line intensities and Q_i is defined by (2.6). Similar expressions can be derived for the cases of polarized electrons and unpolarized atoms, or for both electrons and atoms polarized‡.

An expression for polarization of the alkali doublet radiation at 90 degrees to the electron beam, including all hyperfine structure effects, has been given by Flower and Seaton (1967). They obtain (in percent)

$$P = \frac{100(I_{\parallel} - I_{\perp})}{I_{\parallel} + I_{\perp}} = \frac{300(9\alpha - 2)(Q_0 - Q_1)}{12Q_0 + 24Q_1 + (9\alpha - 2)(Q_0 - Q_1)} \quad (2.30)$$

where the constant α depends on the values of the energy separation of the hyperfine structure state and the radiative transition probability. Following Karule (1970) we adopt the value $\alpha = 0.288$ in the present work.

† There is an error in the definition of these quantities by Rubin *et al.*, and Kleinpoppen; for example, in the latter paper (p 1017) the equation $F_i = 2\pi \int f_i(\theta) \sin \theta d\theta$ should be $|F_i|^2 = 2\pi \int |f_i|^2 \sin \theta d\theta$ with corresponding replacements for $|G_i|^2$ and $|F_i - G_i|^2$. The quantities used in the formulae for the line radiation are then just D_M , E_M and I_M multiplied by the factor k_i/k_f .

‡ The relative transition probability for radiative decay from the $m_j = |3/2|$ and $m_j = |1/2|$ substates of the $^2P_{3/2}$ state with $\Delta m_j = \pm 1, 3:1$, was omitted by Kleinpoppen in the analysis of the line polarization following collisional excitation. Correct expressions may be obtained either by repeating the analysis of the decay processes, but introducing the additional factor $1/3$ multiplying all excitation amplitudes to $j = 3/2$, $m_j = \pm 1/2$ given in table II, III and IV of that paper, or by evaluation of (2.20).

3. Results

3.1. Energies below the excitation threshold

The threshold for excitation of the 3p state of sodium is at 2.10 eV; at incident energies below this only elastic scattering can occur and the results are expressed in terms of phase shifts η_L . A preliminary calculation was performed in the two state (3s–3p) close coupling approximation, and some of the results, for S waves and P waves below 0.08 Ryd, have already been published (Norcross 1971). The effect of adding higher states in the close coupling expansion was then investigated, three state (3s–3p–3d) and four state (3s–3p–4s–3d) calculations being carried out. Results for the first three partial waves are shown in table 1.

Table 1. Phase shifts for electron–sodium scattering calculated in three different approximations

<i>L</i> = 0, singlet				<i>L</i> = 0, triplet			
<i>k</i> ² (Ryd)	3t–3p	3s–3p–3d	3s–3p–4s–3d	<i>k</i> ² (Ryd)	3s–3p	3s–3p–3d	3s–3p–4s–3d
0.00735	–0.7113	–0.7106	–0.7051	0.00735	–0.1982	–0.1949	–0.1939
0.02205	–1.2322	–1.2316	–1.2208	0.02205	–0.5575	–0.5547	–0.5541
0.0588	1.2939	1.2943	1.3215	0.0735	–1.2181	–1.2167	–1.2165
0.0735	1.1433	1.1437	1.1796	0.11761	–1.5532	–1.5522	–1.5516
0.11761	0.8319	0.8331	0.9084	0.14701	1.4173	1.4181	1.4195
0.14701	0.6959	0.7013	0.8392				
<i>L</i> = 1, singlet				<i>L</i> = 1, triplet			
0.00735	0.1510	0.1529	0.1553	0.00735	0.8645	0.8932	0.8981
0.02205	0.2456	0.2501	0.2553	0.02205	–1.4288	–1.4182	–1.4144
0.0735	0.2513	0.2566	0.2579	0.0735	–1.5611	–1.5598	–1.5548
0.14701	0.5884	0.6298	0.6360	0.14701	1.3153	1.3172	1.3272
<i>L</i> = 2, singlet				<i>L</i> = 2, triplet			
0.00735	0.0355	0.0355†	0.0356†	0.00735	0.0352	0.0355†	0.0356†
0.02205	0.1041	0.1062	—	0.02205	0.0991	0.1015	—
0.0735	0.3559	0.3833	0.3843	0.0735	0.2603	—	0.2769
0.11761	0.6373	0.7403	0.7529	0.11761	0.3424	—	0.3719
0.13231	0.7665	0.9355	—	0.13231	0.3627	0.3907	—
0.14701	0.9468	1.2727	1.3046	0.14701	0.3803	0.4109	0.4181

† No exchange calculation.

In order to obtain the cross sections, an infinite sum over *L* must be evaluated, but it is not of course necessary to do a complete four state exchange close coupling calculation for all partial waves; as *L* increases, simpler approximations may be used to obtain the *T* matrix with sufficient accuracy, and the scheme delineated in table 2 was followed. For *L* ≥ 8 the polarization formula (Rosenberg *et al* 1961),

$$\tan \eta_L = \frac{\pi \alpha_a k^2}{(2L+3)(2L+1)(2L-1)} \quad (3.1)$$

was employed, where α_a is the atomic dipole polarizability. Checks were made in each case to ascertain that no significant error was introduced through these different approximations by calculating the partial cross sections in both approximations at the values of *L* where the changes were made. The final results should therefore be

Table 2. Approximations used for different values of L to calculate elastic scattering phase shifts at energies below the excitation threshold

Approximation	Incident energy in eV					
	0.1	0.15	1.0	1.6	2.0	2.05
four state, exchange	0, 1	0, 1	0 to 2	0 to 2	0 to 2	0 to 3
four state, no exchange	2, 3	2 to 4	3, 4	3, 4	3 to 5	4 to 7
two state, no exchange	4 to 7	5 to 7	5 to 7	5 to 7	6, 7	—
polarization formula	≥ 8	≥ 8	≥ 8	≥ 8	≥ 8	≥ 8

the same as if a four state close coupling approximation had been used for each partial wave. Up to 50 partial waves were included in the sum for the total cross sections, and up to 150 for the angular distributions, since the sum (2.7) converges more slowly than do (2.2) or (2.3), especially in the forward and backward directions.

In table A1 (see Appendix) are given the values obtained for the quantities $|f|^2$, $|g|^2$ and $|f-g|^2$, after division by π to put them into units of $\pi a_0^2 \text{ sr}^{-1}$. All of the various differential scattering functions may be readily obtained from this table and the formulae of § 2.2.1. In table 3 are given the values obtained for the total elastic and spin-flip cross sections, as well as the diffusion and viscosity cross sections defined by

$$Q_D = \frac{\pi}{4k_i^2} \sum_{L,S} (L+1)(2S+L) |T_{11}^{S,L} - T_{11}^{S,L+1}|^2 \quad (3.2)$$

and

$$Q_V = \frac{\pi}{4k_i^2} \sum_{L,S} \frac{(L+1)(L+2)}{(2L+3)} (2S+1) |T_{11}^{S,L} - T_{11}^{S,L+2}|^2. \quad (3.3)$$

The two state close coupling results are also given for comparison.

Table 3. Cross sections for elastic scattering of electrons by sodium atoms, in two state (3s-3p) and four state (3s-3p-4s-3d) close coupling approximations, in units of πa_0^2

$E(\text{eV})$	Total elastic		Diffusion		Viscosity		Spin-flip	
	two state	four state	two state	four state	two state	four state	two state	four state
0.1	795.9	835.3	838.5	875.4	338.2	353.6	207.6	219.3
0.15	862.0	873.8	843.5	852.2	370.1	374.8	249.6	254.9
1.0	200.6	204.3	95.9	97.1	86.5	87.6	45.8	45.5
1.6	147.2	155.9	52.1	56.1	51.7	53.7	27.2	29.0
2.0	136.1	151.2	41.0	51.2	42.0	47.0	21.8	30.8
2.05	—	153.2	—	51.7	—	47.7	—	32.0

3.2. Energies above the excitation threshold

Results have also been obtained at four energies (2.2 eV, 3 eV, 4 eV and 5 eV) above the excitation threshold, in the (3s-3p) and (3s-3p-4s-3d) close coupling approximations.

In order to obtain the contributions from large values of L , the following approximations were used for the R matrix elements:

$$R_{11} = \frac{\pi\alpha_d k^2}{(2L+3)(2L+1)(2L-1)} \quad (3.4)$$

which gives good agreement with close coupling at values of L for which excitation is negligible; and for the other elements

$$R_{ij} = -\frac{\pi}{2} \int_0^\infty J_{l_2+1/2}(k_i r) V_{ij}(r) J_{l_2+1/2}(k_f r) r dr \quad (3.5)$$

where V_{ij} is the potential appearing in the close coupling equations. The T matrix was then obtained from (2.1). This is a variant of the unitarized Born approximation (Seaton 1961) and was only used to evaluate the T matrices for $L \geq 12$. The different approximations employed to obtain the different partial wave contributions to the scattering amplitudes and total cross sections are summarized in table 4.

Table 4. Approximations used for the different values of L to calculate T matrices for scattering of electrons by sodium atoms at energies above the first excitation threshold

Approximation	Incident energy in eV			
	2.2	3	4	5
four state, exchange	0 to 3	0 to 3	0 to 4	0 to 5
four state, no exchange	4 to 7	4 to 9	5 to 12	6 to 12
two state, no exchange	8 to 11	10 to 13	—	13 to 18
Born, polarization formula	≥ 12	≥ 14	≥ 13	≥ 19

The squares of the elastic scattering amplitudes are given in table A2, as in table A1. For excitation, we give in table A3 the two sets of amplitudes corresponding to $M = 0$ and $|M| = 1$, multiplied by the factor $k_f/\pi k_i$ so that they may be summed in various combinations to give differential cross sections in units of $\pi a_0^2 \text{sr}^{-1}$. As for elastic scattering, the results of table A3 may be used in conjunction with the formulae of § 2.2.2 to calculate any desired experimental quantity.

Also of interest are the integrated amplitudes D_M , E_M and I_M of (2.26), and these are given in table 5 (again divided by π). Finally, we give in table 6 the total elastic, excitation

Table 5. Partial cross sections defined by equation (2.26) calculated in the two state (3s–3p) and four state (3s–3p–4s–3d) close coupling approximations, in units of πa_0^2

	Energy (eV)							
	2.2		3.0		4.0		5.0	
	two state	four state	two state	four state	two state	four state	two state	four state
D_0	4.937	9.623	12.305	15.819	15.200	17.035	18.374	16.286
E_0	7.038	10.143	9.775	11.828	8.403	7.161	6.091	6.032
I_0	0.474	0.402	15.093	17.781	19.315	19.028	20.695	20.744
D_1	0.563	1.050	4.018	3.213	6.735	5.723	9.544	7.457
E_1	0.569	0.931	1.119	0.386	0.904	0.468	0.963	0.520
I_1	0.053	0.077	3.704	3.065	5.191	5.387	7.380	7.240

Table 6. Total cross sections in units of πa_0^2 calculated in the two state (3s–3p) and four state (3s–3p–4s–3d) close coupling approximations. Also shown is the polarization, P , of the line radiation as calculated in the two approximations from equation (2.30)

Energy (eV)	$Q(3s \rightarrow 3s)$		$Q_{SF}(3s \rightarrow 3s)$		$Q(3s \rightarrow 3p)$		$Q_{SF}(3s \rightarrow 3p)$		$Q(3s \rightarrow 4s)$		$Q(3s \rightarrow 3d)$		$P(\%)$	
	two state	four state	two state	four state	two state	four state	two state	four state	two state	four state	two state	four state	two state	four state
2.2	128.2	121.1	20.5	18.4	7.41	12.14	8.18	12.00	—	—	10.84	10.65		
3.0	87.4	86.0	10.1	8.7	27.43	29.38	12.01	12.60	—	—	7.45	9.46		
4.0	61.3	64.5	7.6	4.8	34.29	33.19	10.21	8.10	2.00	4.68	6.36	6.89		
5.0	47.6	48.9	6.0	3.6	40.47	36.75	8.02	7.07	3.26	5.46	4.91	5.50		

and spin–flip cross sections, and the polarization of the line radiation, which are compared with two state results. Calculations were also performed at several additional energies in the four state approximation only, and these results are given in table A4.

4. Discussion

The phase shifts calculated in the two state approximation are in excellent agreement with those of Karule (1965); and are very similar to those obtained for lithium by Burke and Taylor (1969). A low energy 3P resonance is obtained for both atoms, and there is indication of resonance structure in the 1P and 1D phases in the region of the excitation threshold.

It is seen that, in general, the change in the phase shifts caused by inclusion of higher states is quite small (table 1); inclusion of the 3d state increases S and P wave phases by a small amount; and in the case of the P waves results in a minute shift of the resonances to lower energies. The effect on the 3D partial wave is also small, and the only partial wave to be significantly changed is the 1D wave, the phase shift being increased by a greater extent, especially just below the excitation threshold, resulting in a corresponding shift in the resonance position. When the 4s state is added, a further small increase in the phase shifts results, but this is small except in the case of the 1S partial wave near the excitation threshold. The fact that the inclusion of more states in the expansion leads to increases in phase shifts is in accordance with the bound principles worked out by Percival (1960) and by Hahn *et al* (1964).

At the lower energies, the differential elastic cross sections are strongly peaked in the forward and backward directions, reflecting the dominance of the 3P partial wave, but as the incident energy is increased, the backward scattering peak becomes less marked as the higher partial waves begin to make themselves felt. At energies above about 3 eV, the scattering takes place mainly in the forward direction. These trends are illustrated in figure 1, where the differential cross sections are plotted as a function of scattering angle for several energies. It is also apparent from figure 1 that the difference between the four state and two state results is small, in general, and that at those energies and angles at which significant percentage differences occur, the cross section itself is small. The four state results agree very well with the measurements of Gehenn and Reichert (1972).

The discrepancy between our two state results and those of Karule (1965) might be due to an insufficient number of partial waves being included in the latter calculations.

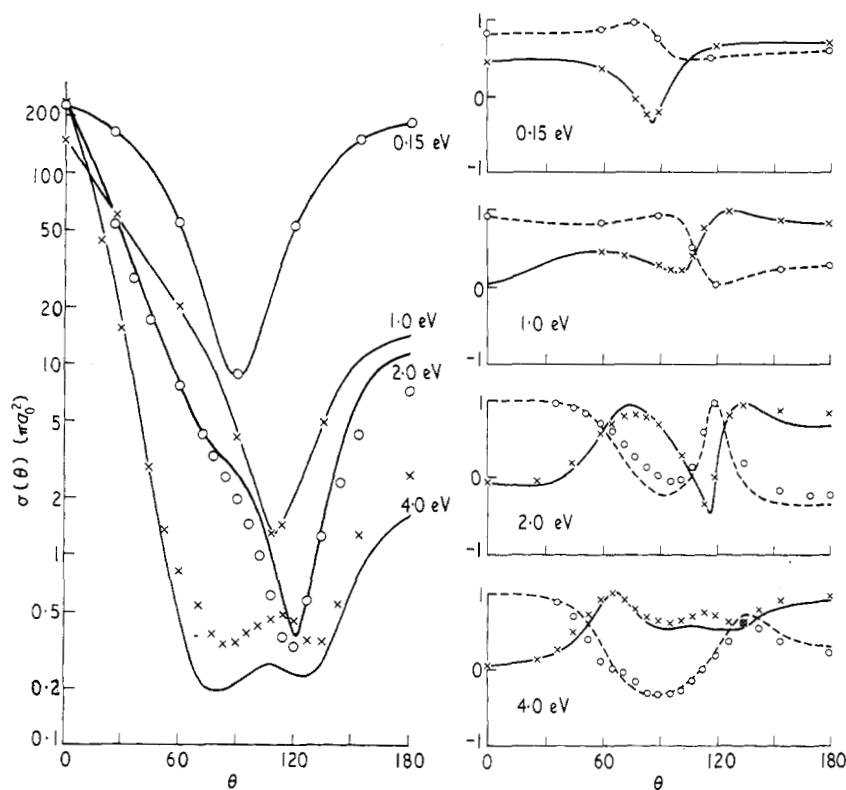


Figure 1. Differential cross section $\sigma(\theta)$, exchange polarization (—) $p(\theta)/k(\theta)$, and direct polarization (---) $n(\theta)/k(\theta)$ for elastic scattering of electrons by sodium. Curves, four state results; \times and \circ , two state results.

As mentioned previously, this will have its greatest effect at small and large angles, which is in fact where the chief discrepancies occur. For example, at 2.2 eV partial waves for $L > 30$ contribute 10% of the differential cross section for scattering at 0° .

Near the 3P resonance in the total elastic scattering cross section at 0.15 eV, the exchange polarization $p(\theta)/k(\theta)$ is fairly large for both the forward and backward scattering peaks in $\sigma(\theta)$, an effect noted by Burke and Taylor (1969) in lithium, and the direct polarization $n(\theta)/k(\theta)$ is fairly large at all angles of scattering. Drukarev and Obyedkov (1971) have remarked that at those low energies where electron scattering from lithium and sodium is nearly isotropic, the exchange polarization $p(\theta)/k(\theta)$ is nearly 100% in all directions. In fact, the exchange polarization in our calculations does not exceed 85% in all directions for lithium or sodium if the electron energy exceeds 1.5 meV.

At energies above the excitation threshold, $p(\theta)/k(\theta)$ shows more complicated structure, rising from a small value at 0° to a peak value of over 95% in the 60° – 80° region, and to another peak in the backward direction. The direct polarization $n(\theta)/k(\theta)$ is large only in the forward direction, and also shows complicated structure. Again, the differences between the four state and two state results are small, except for the structure above 90° for incident energies of 3 eV and greater.

The inelastic differential cross section $\sigma(\theta)$ (2.16) for three energies is shown in figure 2 together with the quantity $R(\theta)$ measured by Rubin *et al* (1969) and Goldstein

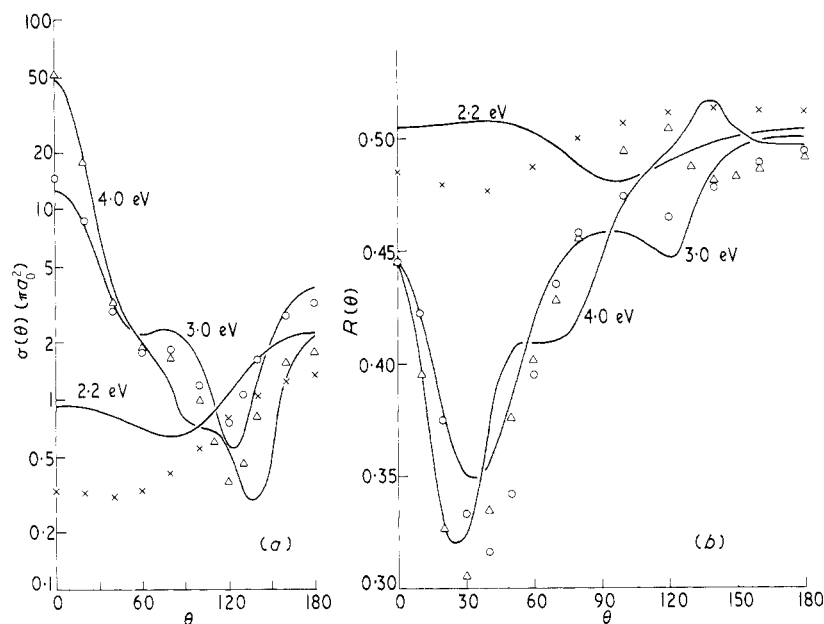


Figure 2. (a) The differential cross sections for excitation of the 3p state of sodium, $\sigma(\theta)$, and (b) the ratio $R(\theta)$ of differential atomic spin exchange to total differential cross sections. Continuous curves, four state results; \times , \circ and \triangle , two state results for 2.2, 3.0 and 4.0 eV, respectively.

et al (1972) for potassium. At 2.2 eV the two state and four state results are seen to differ significantly, due to slight shifts in resonance structure, but the cross sections themselves are small. At higher energies the differences are small, and strong peaking in the forward and backward direction is observed.

It is clear from tables 3 and 6 that the inclusion of the 4s and 3d states has little effect on the total cross sections, except for small differences around 0.15 eV and near the excitation threshold. The elastic cross section rises very rapidly from its threshold to a peak of about $900 \pi a_0^2$ at about 0.13 eV, this peak being due to the 3P resonance, and falls off rapidly to higher energies. There is a cusp at the excitation threshold. The differences between the two state and four state calculations around 2.1 eV are caused by the shift in position of the 1D and 1P resonances.

The cusp in the total elastic scattering cross section at threshold has been observed experimentally by Andrick *et al* (1972), who have measured relative differential elastic scattering cross sections at angles from 20° to 145° as a function of electron energy. Their observation that the cusp occurs most strongly near 105° , and very weakly, if at all, around 60° and 130° , is in very good agreement with the present results. The observed structure is slightly less pronounced, no doubt due partly to finite energy and angular resolution in the experiment. The cusp has been observed by Gehenn and Reichert (1972).

The total cross section, obtained by summing the contributions from $3s \rightarrow 3s$, $3p$, $4s$ and $3d$, is shown graphically in figure 3. At energies above the excitation threshold for the $4p$ state, contributions from transitions to this and higher states, not allowed for in the calculations, ought to be included to obtain the true total cross section. However, at the energies considered the $3s \rightarrow 3s$ and $3s \rightarrow 3p$ contributions are much larger than the others, and the neglected part is probably small. Also shown in figure 3

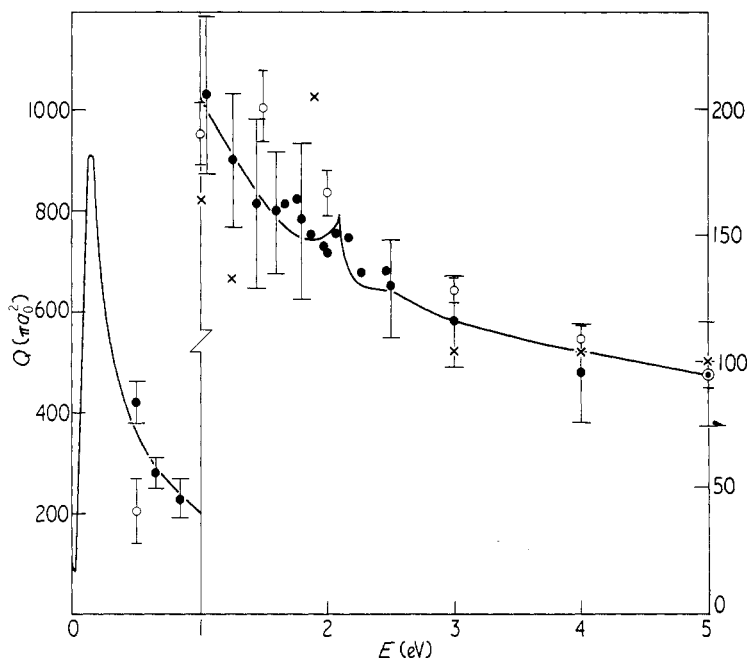


Figure 3. Total cross section for scattering of electrons by sodium. — present results; \times , experiment of Brode (1929) divided by two; \circ , experiment of Perel *et al* (1962) normalized to theory at 5 eV; \bullet experiment of Rubin (1972).

are the experimental points of Brode (1929), which have been divided by two, and it is seen that these results are about a factor of two larger than theory, reflecting the general trend for other electron-alkali cross sections mentioned in the introduction. The relative measurements of Perel *et al* (1962) are also shown; these results have been normalized to the theory at 5 eV for the sake of comparison, and the resulting agreement is very good above 2 eV. Preliminary results from an absolute measurement by Rubin (1972) are in good agreement with the present results.

The $3s \rightarrow 3p$ excitation cross section is plotted in figure 4, together with the results of various other authors. Agreement between theory and the results of Enemark and Gallagher (1972) is seen to be excellent for the four state results and good for the two state results. The experimental results of Zapesochnyi (1967) are about 60% those of Enemark and Gallagher near the maximum. The total cascade correction used in the latter work (Zapesochnyi and Shimon 1965) is $2.4 \pm 0.6\pi a_0^2$ at 4 eV and $5.9 \pm 2.0\pi a_0^2$ at 5 eV, compared with the values obtained for the sum $Q(3s \rightarrow 4s) + Q(3s \rightarrow 3d)$ of 6.7 and $8.7\pi a_0^2$, respectively, from the present work. The energy is too low for meaningful comparison of these two cross sections with the values calculated by Hertel and Rost (1971) and Korff *et al* (1971), respectively, but this suggests that the results of Enemark and Gallagher might be somewhat high at 4 and 5 eV. In view of the neglect of higher states in the present calculation, this is not certain. The differences between the three experimental results shown, and possible explanations, are discussed in detail by Enemark and Gallagher.

The results obtained for the polarization of the line radiation for polarized atoms and unpolarized electrons in the limit when hyperfine structure can be neglected, that is an intermediate magnetic field, using (2.27) and (2.28) are shown in figure 5. The polarization for the unresolved doublet is a fraction whose numerator and denominator are

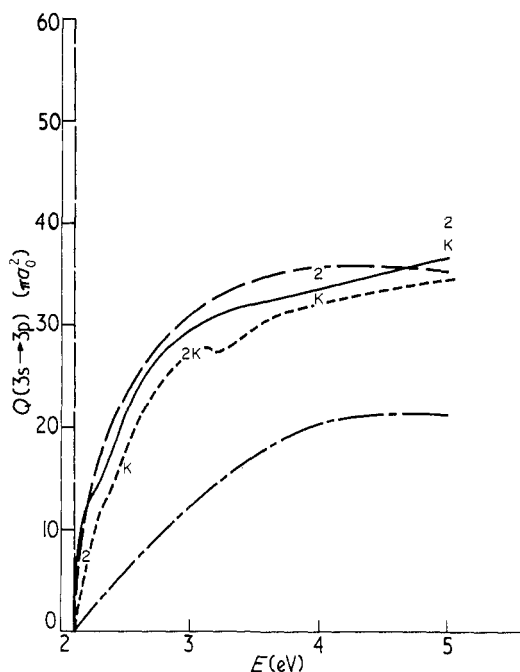


Figure 4. Cross section for excitation of the 3p state of sodium by electron impact. 2, present two state results; — four state results; K, Karule (1965); — — Enemark and Gallagher (1972); - · - Zapesochnyi (1967); - - - Gould (1970).

composed of the sums of the numerators and denominators, respectively, of (2.27) and (2.28). The polarization of the D_1 and D_2 lines and unresolved doublet is consistently higher with the four state than with the two state results, except at 2.2 eV where the latter results are about -1% for all three quantities. This agreement is better than

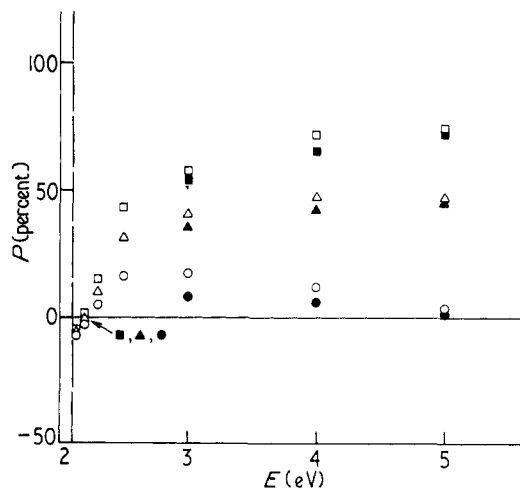


Figure 5. Polarization of the $3p^2P \rightarrow 3s^2S$ line radiation of sodium following electron impact excitation of polarized atoms by unpolarized electrons (equations (2.27) and (2.28)); for the D_1 line, \circ and \bullet ; for the D_2 line, \square and \blacksquare ; and for the unresolved doublet, \triangle and \blacktriangle . The closed symbols are two state results, the open symbols are four state results.

that for the individual partial cross sections, table 5, particularly for the spin-flip cross section for excitation of the $|M| = 1$ state, E_1 , which is most strongly influenced by the shifts in the resonance structure for singlet scattering. The interference cross sections I_0 and I_1 , on the other hand, are in very good agreement for the two approximations, consistent with the small changes in triplet phase shifts below threshold seen in table 1.

The results obtained for the polarization of the line radiation in the low field limit, that is equation (2.30), are shown in figure 6. The four state results generally lie just above the two state results, and are in good agreement with the measurements of Enemark and Gallagher (1972), and Gould (1970), but lie well below the values obtained by Hafner and Kleinpoppen (1967). Cascade corrections were also made in the polarization measurements of Enemark and Gallagher, but these are much less significant (of order 0.1 %) at 4 and 5 eV than the corrections to the measured excitation function.

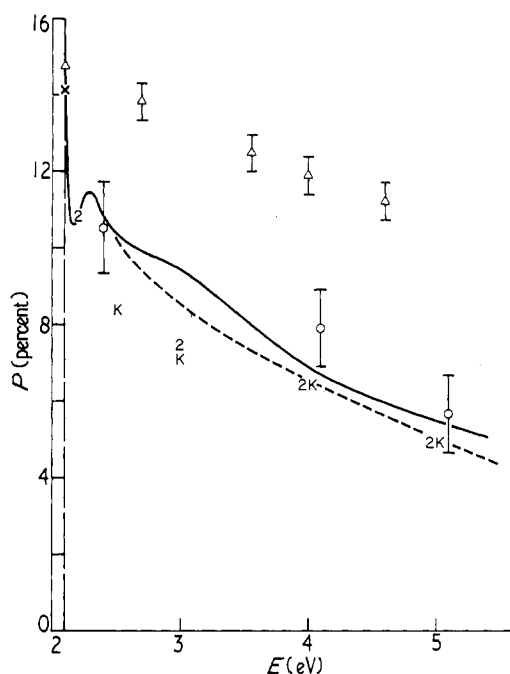


Figure 6. Polarization of the $3p^2P \rightarrow 3s^2S$ line radiation of sodium following electron impact excitation (equation (2.30)). 2, present two state results; ——— four state results; K, Karule (1970); - - - - Enemark and Gallagher (1972); O, Gould (1970); Δ , Hafner and Kleinpoppen (1967). The point X is the threshold value given by Flower and Seaton (1967), which is independent of calculated cross sections.

These results are difficult to understand, for if one takes the case of lithium, the two state calculations by Karule (1970) and Burke and Taylor (1969) yield results lying below the experimental points of Hafner and Kleinpoppen by as much as 15%, but

the subsequent calculations by Feautrier (1970), which attempt to improve the usual two state close coupling approximation by allowing for the full dipole polarizability of both the 2s and 2p states, resolve most of the discrepancy. Now in the case of sodium, a (3s-3p-4s-3d) close coupling calculation ought to take into account most of the dipole polarizability of the 3p state, and should therefore be a reasonably close approximation to a calculation of the type performed by Feautrier; however the results obtained for the polarization of the sodium line radiation in the four state approximation do not succeed in removing the discrepancy between the two state calculations and the experiment of Hafner and Kleinpoppen.

The value obtained for the low-field polarization indicates that both a local maximum and minimum are present, and hence that the polarization drops very steeply from threshold. This possibility of structure has been suggested by Seaton (1966), but never before observed in alkali atoms. This structure is even more pronounced in the polarization of the D_2 line measured separately (that of the D_1 line is zero), the formula for which can be obtained from (2.30) by replacing the factor $12(Q_0 + 2Q_1)$ by $8(Q_0 + 2Q_1)$.

The excitation cross section, figure 4, is also affected slightly, but these features were not observable within the energy resolution (0.3 eV) of the Enemark and Gallagher experiment. Gould (1970) did observe a definite change of slope in the excitation cross section at 2.3 eV. All of this structure is related to the dominance of the 1P and 1D partial waves just above threshold, whereas the triplet contribution to the excitation cross section, for example, increases slowly and exceeds the singlet contribution only above 2.5 eV.

5. Conclusions

The main conclusion to be drawn from this work is that the addition of the 3d and 4s states to the close coupling expansion for scattering of electrons by sodium atoms at energies below 5 eV has generally a small effect on total cross sections, and hence that disagreement between earlier theoretical cross sections and the experiment of Brode (1929), and between calculated polarization of the line radiation and the experiment of Hafner and Kleinpoppen (1967), cannot be attributed to lack of convergence in the close coupling calculations. Additional calculations of the present type for lithium, and using the method of Feautrier for sodium, obviously seem warranted.

At some angles and energies, the four state calculations give angular distributions which differ noticeably from the two state results; essential agreement is obtained with the 3s \rightarrow 3p excitation cross section and line polarization measured by Enemark and Gallagher (1972) and independently by Gould (1970) and it would be reasonable to conclude that our elastic scattering results are quite reliable. Additional confirmation is provided by the results of measurements of the differential elastic scattering cross section by Andrick *et al* (1972) and Gehenn and Reichert (1972), and the total cross section by Rubin (1972).

This paper has been devoted exclusively to processes related to electron collisions with the ground state. Additional calculations will be performed in the same approximation (four state close coupling) to obtain rates for elastic scattering from, and collisional transitions between the fine structure states of, the 3p state, and for excitation of the 4s and 3d states from the 3p state. It is expected that these rates will also be strongly affected by the resonant singlet feature near the 3p threshold.

Acknowledgments

Most of the computations involved in this work were performed on the IBM 360/65 computer at University College London, with some assistance from Mr J Wells. They were completed through the courtesy of the NASA Goddard Space Flight Center, Greenbelt, Maryland. We would like to acknowledge several stimulating discussions with, and encouragement from, Dr M V McCusker, Dr E Enemark and Dr A Gallagher, and to thank Dr H Hofmann, Professor Dr E Reichert and Dr K Rubin for communicating their results in advance of publication. This work was partially supported by the National Science Foundation through Grant No. GP-17174.

Appendix

Table A1. Squares of the scattering amplitudes for elastic scattering of electrons by sodium, in units of πa_0^2

θ	$ f ^2$	$ g ^2$	$ f-g ^2$	θ	$ f ^2$	$ g ^2$	$ f-g ^2$
<i>E</i> = 0.1 (eV)				<i>E</i> = 0.15 (eV)			
0.00	1.1512+02†	3.9161+01	2.8856+02	0.00	1.145+02	3.7073+01	2.8868+02
10.00	9.9048+01	3.7938+01	2.5918+02	10.00	1.05+02	3.5726+01	2.6812+02
20.00	8.1719+01	3.4429+01	2.2069+02	20.00	9.754+01	3.1874+01	2.3679+02
30.00	6.4384+01	2.9090+01	1.7668+02	30.00	7.9963+01	2.6060+01	1.9722+02
40.00	4.7957+01	2.2617+01	1.3077+02	40.00	6.3920+01	1.9118+01	1.5277+02
50.00	3.3425+01	1.5863+01	8.6987+01	50.00	4.8456+01	1.2059+01	1.0769+02
60.00	2.1719+01	9.7329+00	4.9324+01	60.00	3.4533+01	5.9540+00	6.6548+01
70.00	1.3597+01	5.0683+00	2.1273+01	70.00	2.3084+01	1.7906+00	3.3605+01
80.00	9.5484+00	2.5460+00	5.4066+00	80.00	1.4875+01	3.5015-01	1.2280+01
90.00	9.7288+00	2.5919+00	3.0826+00	90.00	1.0388+01	2.1036+00	4.7210+00
100.00	1.3929+01	5.3260+00	1.4270+01	100.00	9.7439+00	7.1462+00	1.1525+01
110.00	2.1580+01	1.0544+01	3.7532+01	110.00	1.2668+01	1.5176+01	3.1647+01
120.00	3.1801+01	1.7738+01	7.0160+01	120.00	1.8517+01	2.5522+01	6.2515+01
130.00	4.3479+01	2.6154+01	1.0846+02	130.00	2.6350+01	3.7216+01	1.0033+02
140.00	5.5372+01	3.4881+01	1.4815+02	140.00	3.5034+01	4.9098+01	1.4050+02
150.00	6.6226+01	4.2954+01	1.8480+02	150.00	4.3376+01	5.9954+01	1.7818+02
160.00	7.4901+01	4.9473+01	2.1434+02	160.00	5.0261+01	6.8650+01	2.0887+02
170.00	8.0493+01	5.3704+01	2.3348+02	170.00	5.4784+01	7.4268+01	2.2887+02
180.00	8.2422+01	5.5170+01	2.4010+02	180.00	5.6358+01	7.6210+01	2.3582+02
<i>E</i> = 1.0 (eV)				<i>E</i> = 1.6 (eV)			
0.00	1.4869+02	1.0629+01	1.5267+02	0.00	2.1824+02	3.3206+00	1.9796+02
10.00	9.3572+01	1.0354+01	1.0860+02	10.00	1.3062+02	3.2800+00	1.2217+02
20.00	5.8111+01	9.5578+00	8.0168+01	20.00	7.4519+01	3.1793+00	7.6083+01
30.00	3.6655+01	8.3274+00	6.1356+01	30.00	4.0846+01	3.0647+00	4.9212+01
40.00	2.3773+01	6.7928+00	4.7445+01	40.00	2.1242+01	2.9674+00	3.2938+01
50.00	1.5985+01	5.1125+00	3.6022+01	50.00	1.0445+01	2.8671+00	2.2375+01
60.00	1.1096+01	3.4578+00	2.6099+01	60.00	5.0013+00	2.6863+00	1.4944+01
70.00	7.7633+00	1.9988+00	1.7497+01	70.00	2.5464+00	2.3285+00	9.4124+00
80.00	5.2558+00	8.9313-01	1.0451+01	80.00	1.5249+00	1.7465+00	5.3024+00
90.00	3.2639+00	2.7435-01	5.2909+00	90.00	1.0289+00	1.0088+00	2.4769+00
100.00	1.7149+00	2.3721-01	2.2204+00	100.00	6.3889-01	3.2484-01	8.6089-01
110.00	6.4025-01	8.2057-01	1.2183+00	110.00	2.7377-01	4.6909-03	3.2045-01
120.00	8.6948-02	1.9901+00	2.0330+00	120.00	4.3927-02	3.5597-01	6.4624-01
130.00	5.0340-02	3.6274+00	4.2175+00	130.00	9.7115-02	1.5538+00	1.5730+00

Table A1—continued

θ	$ f ^2$	$ g ^2$	$ f-g ^2$	θ	$ f ^2$	$ g ^2$	$ f-g ^2$
<i>E</i> = 1.0 (eV) continued				<i>E</i> = 1.6 (eV) continued			
140.00	4.3864−01	5.5324+00	7.1929+00	140.00	4.9647−01	3.5361+00	2.8131+00
150.00	1.0822+00	7.4436+00	1.0336+01	150.00	1.1709+00	5.9745+00	4.0946+00
160.00	1.7703+00	9.0775+00	1.3068+01	160.00	1.9321+00	8.3417+00	5.1892+00
170.00	2.2925+00	1.0178+01	1.4917+01	170.00	2.5339+00	1.0062+01	5.9224+00
180.00	2.4881+00	1.0566+01	1.5571+01	180.00	2.7640+00	1.0691+01	6.1808+00
<i>E</i> = 2.0 (eV)				<i>E</i> = 2.05 (eV)			
0.00	2.5651+02	1.5854+00	2.2721+02	0.00	2.5499+02	2.8424+00	2.3402+02
10.00	1.5592+02	1.3457+00	1.3182+02	10.00	1.5620+02	2.4464+00	1.3506+02
20.00	9.0876+01	7.8851−01	7.5009+01	20.00	9.2515+01	1.4814+00	7.5843+01
30.00	5.0280+01	3.0914−01	4.3533+01	30.00	5.2343+01	4.9937−01	4.3132+01
40.00	2.5214+01	3.0995−01	2.6163+01	40.00	2.6899+01	9.0448−02	2.5346+01
50.00	1.0622+01	9.5871−01	1.6248+01	50.00	1.1547+01	5.6372−01	1.5456+01
60.00	3.2359+00	2.0617+00	1.0144+01	60.00	3.4743+00	1.7640+00	9.5492+00
70.00	4.9343−01	3.1280+00	6.0496+00	70.00	3.8633−01	3.1241+00	5.6726+00
80.00	2.3802−01	3.6059+00	3.2124+00	80.00	1.3718−01	3.9391+00	3.0017+00
90.00	7.9493−01	3.1827+00	1.3645+00	90.00	8.8637−01	3.7350+00	1.2541+00
100.00	1.1319+00	1.9983+00	3.7303−01	100.00	1.4021+00	2.5541+00	3.1510−01
110.00	9.1848−01	6.5562−01	9.7894−02	110.00	1.2300+00	1.0059+00	6.1815−02
120.00	3.8525−01	1.8814−03	3.6801−01	120.00	5.9525−01	4.0586−02	3.2834−01
130.00	1.5872−02	7.6216−01	9.9573−01	130.00	7.0727−02	5.2981−01	9.3221−01
140.00	2.0583−01	3.1848+00	1.7974+00	140.00	1.6526−01	2.8400+00	1.7043+00
150.00	1.0294+00	6.8621+00	2.6105+00	150.00	1.0155+00	6.5962+00	2.4984+00
160.00	2.1981+00	1.0820+01	3.3007+00	160.00	2.3099+00	1.0759+01	3.1858+00
170.00	3.2103+00	1.3858+01	3.7624+00	170.00	3.4600+00	1.4001+01	3.6537+00
180.00	3.6085+00	1.4995+01	3.9252+00	180.00	3.9165+00	1.5223+01	3.8202+00

† Here, and in the subsequent tables, the quantity following the last decimal place is the power of ten by which the entry must be multiplied.

Table A2. Squares of the scattering amplitudes for elastic scattering of electrons by sodium, in units of πa_0^2

θ	$ f ^2$	$ g ^2$	$ f-g ^2$	θ	$ f ^2$	$ g ^2$	$ f-g ^2$
<i>E</i> = 2.2 (eV)				<i>E</i> = 3.0 (eV)			
0.0	1.930+02	4.860+00	2.485+02	0.0	2.342+02	1.082+00	2.671+02
10.0	1.069+02	4.420+00	1.421+02	10.0	1.177+02	1.079+00	1.411+02
20.0	5.848+01	3.286+00	7.750+01	20.0	5.319+01	1.061+00	6.849+01
30.0	3.256+01	1.933+00	4.201+01	30.0	2.212+01	1.005+00	3.131+01
40.0	1.796+01	8.900−01	2.327+01	40.0	8.252+00	8.945−01	1.337+01
50.0	9.167+00	4.975−01	1.346+01	50.0	2.581+00	7.417−01	5.293+00
60.0	3.873+00	7.576−01	8.042+00	60.0	5.660−01	5.973−01	1.985+00
70.0	1.090+00	1.361+00	4.695+00	70.0	4.136−02	5.271−01	7.686−01
80.0	1.202−01	1.862+00	2.445+00	80.0	2.060−02	5.583−01	3.645−01
90.0	1.979−01	1.917+00	9.823−01	90.0	9.370−02	6.369−01	2.432−01
100.0	5.710−01	1.457+00	2.078−01	100.0	1.281−01	6.479−01	2.002−01
110.0	7.242−01	7.304−01	1.605−02	110.0	1.185−01	5.081−01	1.463−01
120.0	5.294−01	1.852−01	2.560−01	120.0	9.355−02	2.709−01	1.020−01
130.0	1.964−01	2.517−01	7.805−01	130.0	7.756−02	1.470−01	2.325−01
140.0	5.036−02	1.131+00	1.477+00	140.0	7.986−02	3.903−01	7.811−01
150.0	2.811−01	2.680+00	2.245+00	150.0	9.846−02	1.105+00	1.862+00

Table A2—continued

θ	$ f ^2$	$ g ^2$	$ f-g ^2$	θ	$ f ^2$	$ g ^2$	$ f-g ^2$
<i>E</i> = 2.2 (eV) continued				<i>E</i> = 3.0 (eV) continued			
160.0	8.127−01	4.444+00	2.964+00	160.0	1.261−01	2.115+00	3.269+00
170.0	1.353+00	5.835+00	3.484+00	170.0	1.500−01	3.010+00	4.485+00
180.0	1.578+00	6.361+00	3.675+00	180.0	1.592−01	3.367+00	4.965+00
<i>E</i> = 4.0 (eV)				<i>E</i> = 5.0 (eV)			
0.0	2.480+02	1.320+00	2.809+02	0.0	2.506+02	9.726−01	2.705+02
10.0	1.137+02	1.272+00	1.331+02	10.0	1.028+02	9.468−01	1.119+02
20.0	4.385+01	1.137+00	5.356+01	20.0	3.346+01	8.715−01	3.685+01
30.0	1.468+01	9.372−01	1.910+01	30.0	9.215+00	7.550−01	1.064+01
40.0	4.097+00	7.085−01	6.136+00	40.0	2.046+00	6.144−01	2.931+00
50.0	8.291−01	4.947−01	1.839+00	50.0	2.901−01	4.712−01	9.378−01
60.0	7.024−02	3.361−01	5.791−01	60.0	3.903−03	3.442−01	3.890−01
70.0	6.802−03	2.553−01	2.043−01	70.0	3.332−02	2.460−01	1.482−01
80.0	6.054−02	2.475−01	7.485−02	80.0	9.061−02	1.865−01	2.374−02
90.0	9.847−02	2.802−01	4.718−02	90.0	1.233−01	1.693−01	2.345−02
100.0	1.105−01	3.038−01	7.752−02	100.0	1.315−01	1.786−01	1.240−01
110.0	1.117−01	2.738−01	1.280−01	110.0	1.231−01	1.802−01	2.452−01
120.0	1.142−01	1.846−01	1.765−01	120.0	1.080−01	1.485−01	3.098−01
130.0	1.195−01	9.406−02	2.656−01	130.0	9.405−02	9.663−02	3.179−01
140.0	1.307−01	1.072−01	4.681−01	140.0	8.708−02	7.332−02	3.201−01
150.0	1.471−01	3.034−01	8.390−01	150.0	8.787−02	1.234−01	3.624−01
160.0	1.633−01	6.510−01	1.314+00	160.0	9.559−02	2.434−01	4.448−01
170.0	1.771−01	9.919−01	1.739+00	170.0	1.047−01	3.714−01	5.221−01
180.0	1.831−01	1.134+00	1.921+00	180.0	1.092−01	4.265−01	5.619−01

Table A3. Squares of the scattering amplitudes for excitation of the $M = 0$ and $|M| = 1$ substates of the 3p state of sodium by electron impact, in units of πa_0^2

θ	$ f_0 ^2$	$ g_0 ^2$	$ f_0 - g_0 ^2$	$ f_1 ^2$	$ g_1 ^2$	$ f_1 - g_1 ^2$
<i>E</i> = 2.2 (eV)						
0.0	7.507−01	1.004+00	8.116−02	0	0	0
10.0	7.457−01	9.822−01	7.115−02	3.422−03	6.663−03	1.727−03
20.0	7.324−01	9.177−01	4.607−02	1.316−02	2.499−02	5.630−03
30.0	7.112−01	8.158−01	1.910−02	2.791−02	5.061−02	9.012−03
40.0	6.779−01	6.862−01	3.418−03	4.631−02	7.783−02	9.677−03
50.0	6.303−01	5.442−01	3.207−03	6.730−02	1.013−01	7.306−03
60.0	5.729−01	4.116−01	1.353−02	8.915−02	1.170−01	3.602−03
70.0	5.153−01	3.146−01	2.464−02	1.089−01	1.230−01	7.504−04
80.0	4.754−01	2.803−01	2.813−02	1.232−01	1.191−01	6.001−05
90.0	4.764−01	3.295−01	2.228−02	1.292−01	1.069−01	1.705−03
100.0	5.350−01	4.716−01	1.131−02	1.258−01	8.923−02	4.922−03
110.0	6.561−01	7.005−01	3.351−03	1.142−01	6.939−02	8.632−03
120.0	8.354−01	9.956−01	7.764−03	9.646−02	5.041−02	1.162−02
130.0	1.056+00	1.326+00	2.969−02	7.459−02	3.422−02	1.261−02
140.0	1.292+00	1.656+00	6.792−02	5.182−02	2.149−02	1.125−02
150.0	1.514+00	1.951+00	1.158−01	3.128−02	1.202−02	8.223−03
160.0	1.695+00	2.184+00	1.623−01	1.479−02	5.376−03	4.465−03
170.0	1.814+00	2.332+00	1.961−01	3.851−03	1.358−03	1.268−03
180.0	1.855+00	2.382+00	2.085−01	0	0	0

Table A3—continued

θ	$ f_0 ^2$	$ g_0 ^2$	$ f_0 - g_0 ^2$	$ f_1 ^2$	$ g_1 ^2$	$ f_1 - g_1 ^2$
<i>E</i> = 3.0 (eV)						
0.0	1.423 + 01	2.699 - 01	1.105 + 01	0	0	0
10.0	1.136 + 01	2.524 - 01	8.642 + 00	6.056 - 01	1.076 - 05	6.086 - 01
20.0	6.477 + 00	2.209 - 01	4.607 + 00	1.258 + 00	1.910 - 05	1.260 + 00
30.0	3.476 + 00	2.296 - 01	2.142 + 00	1.133 + 00	6.866 - 04	1.109 + 00
40.0	2.261 + 00	3.392 - 01	1.121 + 00	7.315 - 01	3.974 - 03	6.570 - 01
50.0	1.793 + 00	5.776 - 01	8.291 - 01	4.559 - 01	1.160 - 02	3.296 - 01
60.0	1.507 + 00	9.030 - 01	9.475 - 01	3.260 - 01	2.264 - 02	1.781 - 01
70.0	1.244 + 00	1.199 + 00	1.301 + 00	2.553 - 01	3.344 - 02	1.270 - 01
80.0	9.831 - 01	1.320 + 00	1.627 + 00	1.920 - 01	4.040 - 02	1.124 - 01
90.0	7.391 - 01	1.183 + 00	1.662 + 00	1.282 - 01	4.273 - 02	1.055 - 01
100.0	5.336 - 01	8.375 - 01	1.309 + 00	7.446 - 02	4.239 - 02	1.021 - 01
110.0	3.672 - 01	4.692 - 01	7.293 - 01	3.926 - 02	4.216 - 02	1.050 - 01
120.0	2.366 - 01	3.182 - 01	2.638 - 01	2.311 - 02	4.341 - 02	1.143 - 01
130.0	1.424 - 01	5.553 - 01	2.311 - 01	1.955 - 02	4.499 - 02	1.232 - 01
140.0	8.254 - 02	1.195 + 00	7.420 - 01	1.974 - 02	4.339 - 02	1.201 - 01
150.0	5.004 - 02	2.089 + 00	1.653 + 00	1.730 - 02	3.513 - 02	9.673 - 02
160.0	3.519 - 02	2.993 + 00	2.655 + 00	1.073 - 02	2.066 - 02	5.645 - 02
170.0	2.955 - 02	3.656 + 00	3.418 + 00	3.260 - 03	6.150 - 03	1.673 - 02
180.0	2.813 - 02	3.899 + 00	3.702 + 00	0	0	0
<i>E</i> = 4.0 (eV)						
0.0	5.364 + 01	5.320 - 01	4.352 + 01	0	0	0
10.0	3.237 + 01	5.505 - 01	2.448 + 01	4.433 + 00	3.260 - 03	4.201 + 00
20.0	1.061 + 01	5.990 - 01	6.471 + 00	5.045 + 00	1.203 - 02	4.564 + 00
30.0	3.812 + 00	6.555 - 01	2.263 + 00	2.422 + 00	2.394 - 02	1.983 + 00
40.0	1.893 + 00	6.883 - 01	1.897 + 00	8.622 - 01	3.555 - 02	6.364 - 01
50.0	1.153 + 00	6.727 - 01	1.890 + 00	3.610 - 01	4.207 - 02	3.345 - 01
60.0	7.507 - 01	6.112 - 01	1.661 + 00	2.371 - 01	4.048 - 02	3.050 - 01
70.0	4.368 - 01	5.389 - 01	1.186 + 00	1.780 - 01	3.434 - 02	2.465 - 01
80.0	2.180 - 01	5.047 - 01	7.530 - 01	1.259 - 01	3.236 - 02	1.645 - 01
90.0	8.526 - 02	5.301 - 01	5.196 - 01	8.051 - 02	3.931 - 02	1.025 - 01
100.0	3.249 - 02	5.751 - 01	4.753 - 01	5.244 - 02	5.010 - 02	7.920 - 02
110.0	1.352 - 02	5.562 - 01	4.663 - 01	3.185 - 02	5.495 - 02	6.773 - 02
120.0	9.574 - 03	4.291 - 01	3.615 - 01	1.649 - 02	4.990 - 02	5.113 - 02
130.0	7.397 - 03	2.718 - 01	2.162 - 01	7.273 - 03	4.018 - 02	2.860 - 02
140.0	3.536 - 03	2.713 - 01	2.229 - 01	8.540 - 03	3.255 - 02	1.156 - 02
150.0	6.179 - 03	5.853 - 01	5.720 - 01	1.427 - 02	2.662 - 02	4.105 - 03
160.0	2.708 - 02	1.174 + 00	1.229 + 00	1.376 - 02	1.741 - 02	2.575 - 03
170.0	6.539 - 02	1.763 + 00	1.884 + 00	5.478 - 03	5.695 - 03	8.764 - 04
180.0	8.022 - 02	2.012 + 00	2.167 + 00	0	0	0
<i>E</i> = 5.0 (eV)						
0.0	1.026 + 02	3.283 - 01	9.175 + 01	0	0	0
10.0	4.186 + 01	3.454 - 01	3.524 + 01	1.137 + 01	6.081 - 03	1.088 + 01
20.0	8.164 + 00	3.932 - 01	6.261 + 00	7.712 + 00	2.421 - 02	6.983 + 00
30.0	2.440 + 00	4.599 - 01	2.651 + 00	2.470 + 00	5.213 - 02	1.992 + 00
40.0	1.157 + 00	5.262 - 01	2.105 + 00	6.576 - 01	8.196 - 02	5.261 - 01
50.0	6.063 - 01	5.751 - 01	1.696 + 00	2.348 - 01	1.009 - 01	3.392 - 01
60.0	3.073 - 01	6.040 - 01	1.288 + 00	1.483 - 01	9.883 - 02	3.367 - 01
70.0	1.549 - 01	6.182 - 01	9.592 - 01	1.138 - 01	7.651 - 02	2.720 - 01
80.0	7.701 - 02	6.109 - 01	7.035 - 01	7.747 - 02	4.723 - 02	1.583 - 01
90.0	3.949 - 02	5.694 - 01	4.992 - 01	4.425 - 02	2.633 - 02	6.551 - 02
100.0	1.929 - 02	5.038 - 01	3.578 - 01	2.039 - 02	1.776 - 02	1.907 - 02
110.0	8.082 - 03	4.333 - 01	3.275 - 01	8.657 - 03	1.483 - 02	6.301 - 03

Table A3—continued

θ	$ f_0 ^2$	$ g_0 ^2$	$ f_0 - g_0 ^2$	$ f_1 ^2$	$ g_1 ^2$	$ f_1 - g_1 ^2$
$E = 5.0$ (eV) continued						
120.0	4.403-03	3.520-01	3.618-01	5.236-03	1.292-02	3.751-03
130.0	1.014-02	2.584-01	3.699-01	7.814-03	1.348-02	2.450-03
140.0	2.304-02	2.122-01	3.265-01	1.583-02	1.674-02	2.565-03
150.0	3.724-02	2.994-01	3.291-01	2.370-02	1.822-02	3.505-03
160.0	4.910-02	5.242-01	4.490-01	2.082-02	1.351-02	2.630-03
170.0	5.609-02	7.678-01	6.140-01	8.058-03	4.647-03	8.900-04
180.0	5.899-02	8.728-01	6.875-01	0	0	0

Table A4. As tables 5 and 6 for additional energies, calculated in the four state close coupling approximations

	Energy (eV)				
	2.13	2.16	2.30	2.50	2.70
D_0	5.783	7.891	12.095	14.387	15.439
E_0	6.914	8.766	11.340	11.192	11.813
I_0	0.129	0.182	1.981	9.368	15.418
D_1	0.443	0.886	0.874	1.587	2.408
E_1	0.427	0.826	0.620	0.569	0.482
I_1	0.005	0.024	0.412	1.780	2.639
$Q(3s \rightarrow 3s)$	139.5	129.7	115.3	106.8	97.78
$Q_{sf}(3s \rightarrow 3s)$	29.90	23.57	13.87	11.67	10.44
$Q(3s \rightarrow 3p)$	7.29	10.15	14.61	21.41	26.86
$Q_{sf}(3s \rightarrow 3p)$	7.77	10.42	12.58	12.33	12.78
$P\%$	11.66	10.62	11.45	10.35	9.89

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