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Elastic scattering of electrons by oxygen and nitrogen at intermediate energies

M. Blaha
Department of Physics and Astronomy, University of Maryland, College Park, Maryland 20742

J. Davis
Plasma Physics Division, Naval Research Laboratory, Washington, D. C. 20375

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The total and differential elastic scattering cross section of electrons by atomic oxygen and nitrogen is calculated for energies between 1 and 500 eV in the distorted-wave (DW) approximation. The DW method has been modified by the inclusion of a polarization potential with an adjustable cutoff parameter which is determined variationally. The relative importance of polarization and exchange effects are compared for a variety of energies. These calculations show that the DW method is reliable above about 10 eV and with the inclusion of the polarization potential improves the estimates even below this energy.

I. INTRODUCTION

The occurrence of natural auroral and/or man-made regions of enhanced atmospheric ionization provide a unique means of studying the response of the atmosphere to the deposition of energetic electrons. The electrons upon entering and interacting with the atmospheric constituents exchange energy through inelastic collisional processes and local plasma heating. The result of this energy exhange usually manifests itself in a spectacular visual display of auroral emissions. These emissions provide the necessary information for understanding the complex of mechanisms occurring in the disturbed atmosphere.

The path actually traversed by these incident electrons is determined principally by elastic collisions in which there is very little energy exchanged in a single encounter with the atmospheric constituents. It is clear that knowledge of these atomic parameters for both types of encounters is essential for the construction of reliable energy-deposition rate profiles as well as height profiles of the auroral light emissions.

A survey of the existing total and differential cross-section data reveals that both the experimental and theoretical results are too restrictive in energy and almost entirely omit the important region of intermediate energies, i.e., 10–500 eV. In the absence of reliable estimates of these quantities, many problems of contemporary auroral physics are done in a very approximate and often unsatisfactory fashion.

The purpose of this investigation is to provide estimates of the total and differential elastic-scattering cross sections for atomic oxygen and nitrogen over a fairly broad range of incident-electron energies for application to auroral-deposition problems. The calculations are performed in the distorted wave (DW) approximation. In addition, the DW method is modified by the inclusion of a polarization potential. Finally, the relative importance of exchange and polarization are compared, and a comparison is made with the available experimental and theoretical estimates.

II. METHOD OF CALCULATION

The elastic cross section is calculated in the DW approximation described by Saraph *et al.*[1] and by Eissner and Seaton.[2] However, our approximation differs from theirs in two respects: first, in order to satisfy the orthogonality condition for the free-electron orbitals, we use Lagrange multipliers in the radial equation for the colliding electron, and second, we introduce a polarization potential in which the cutoff parameter r_d is determined variationally.

We consider the elastic scattering by an atom in the state $1s^2 2s^2 2p^q\, SL$. Let $\Phi(1s^2 2s^2 2p^q\, SL,\ l,\ S^T L^T M_S^T M_L^T)$ be the wave function of the total system consisting of an atom in the state SL and a colliding electron with orbital angular momentum l. Φ is antisymmetric in all $q+5$ electrons and in our approximation, Φ is constructed in the usual way from one-electron orbitals containing radial functions P_{nl} for the atomic electrons, which are solutions of Hartree-Fock equations for a single configuration $1s^2\, 2s^2\, 2p^q$, and radial functions F_{kl} for the colliding electron. The F_{kl} are solutions of the equation

$$\left(\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} + \frac{2Z}{r} - 4y_0(P_{1s}^2, r) - 4y_0(P_{2s}^2, r) - 2q\, y_0(P_{2p}^2, r) - 2V_p(r) + k^2\right) F_{kl}(r)$$
$$+ \delta(l,0)\mu_{1s} P_{1s}(r) + \delta(l,0)\mu_{2s} P_{2s}(r) + \delta(l,1)\mu_{2p} P_{2p}(r) = 0, \quad (1)$$

with the asymptotic form

$$F_{kl} \sim k^{-1/2}\sin(kr - \tfrac{1}{2}\pi l + \eta),$$

where η is the phase shift, Z is the nuclear charge, k^2 the energy of the colliding electron in Ry, q is the number of atomic electrons in the $2p$ shell, and the Lagrange multipliers μ are introduced to satisfy the orthogonality of P_{nl} and F_{kl}. (If not specified otherwise, atomic units are used throughout the paper.) Functions y_λ are defined by Saraph *et al.*[1] and by Eissner and Seaton.[2] $V_p(r)$ is a polarization potential for which we adopt either of the forms

$$V_p = -(\alpha_d/2r^4)\{1 - \exp[-(r/r_d)^6]\}, \tag{2}$$

$$V_p = -\tfrac{1}{2}\alpha_d(r_d^2 + r^2)^{-2}. \tag{3}$$

The cutoff parameter r_d will be determined from a variational principle, and α_d is the static dipole polarizibility of the atom. For small r, the potential (2) behaves like r^2, while (3) approaches a constant value.

The restriction imposed upon Φ by the requirement of orthogonality of F_{kl} and P_{2p} can be removed if the complete wave function Ψ of the system contains an "atomic term" representing a capture of the colliding electron to the $2p$ orbital. We therefore adopt Ψ in the form

$$\begin{aligned}\Psi(SL, l, S^TL^TM_S^TM_L^T) = {} & \Phi(1s^2\,2s^2\,2p^q\,SL, l, S^TL^TM_S^TM_L^T) \\ & + c\,\delta(l,1)\delta(L^T, L^a)\delta(S^T, S^a)\delta(M_L^T, M_L^a)\delta(M_S^T, M_S^a)\,\Phi(1s^2\,2s^2\,2p^{q+1}S^aL^aM_S^aM_L^a).\end{aligned} \tag{4}$$

Atomic orbitals in both $\Phi(1s^2\,2s^2\,2p^{q+1}S^aL^a)$ and $\Phi(1s^2\,2s^2\,2p^q\,SL, l, S^TL^T)$ are identical. The parameter c is determined from the condition

$$\frac{\partial}{\partial c}\mathfrak{L}(SL\,ll'\,S^TL^T) = 0, \tag{5}$$

with

$$\mathfrak{L}(SL\,ll'\,S^TL^T) \equiv \langle\Psi(SL, l, S^TL^TM_S^TM_L^T)|H - E|\Psi(SL, l', S^TL^TM_S^TM_L^T)\rangle. \tag{6}$$

H is the Hamiltonian of the total system, E is the total energy, and Ψ is defined by (4). The condition (5) leads to the result (for ground states of O and N)

$$\begin{aligned}\mathfrak{L}(SL\,ll'S^TL^T) = {} & \langle\Phi(1s^2\,2s^2\,2p^q\,SL, l, S^TL^T)|H - E|\Phi(1s^2\,2s^2\,2p^q\,SL, l', S^TL^T)\rangle \\ & - \delta(l,1)\delta(l',1)\delta(L^TL^a)\delta(S^T, S^a)(q+1)(p^qSLpS^aL^a]p^{q+1}S^aL^a)^2 \\ & \times\left(-\tfrac{1}{2}\mu_{2p} + \int P_{2p}V_pF_{kl}\,dr + Q(SL, S^aL^a)R_2(P_{2p}^3F_{kl}) + \tfrac{1}{3}R_1(P_{1s}^2P_{2p}F_{kl}) + \tfrac{1}{3}R_1(P_{2s}^2P_{2p}F_{kl})\right)^2 \\ & [E'(1s^2\,2s^2\,2p^{q+1}S^aL^a) - E'(1s^2\,2s^2\,2p^q\,SL) - \tfrac{1}{2}k^2]^{-1},\end{aligned} \tag{7}$$

where $(p^qSLpS^aL^a]p^{q+1}S^aL^a)$ is the coefficient of fractional parentage, V_p is given by (2) or (3), μ_{2p} is found from the solution of (1), and the radial integrals R_λ are defined in Ref. 1. E' are the expectation values for energies of the corresponding configurations, calculated in both cases from the same orbital basis. For the scattering from the ground state,

$S^aL^a \equiv {}^2P$ and $Q(SL, S^aL^a) = \frac{1}{5}$ for oxygen,

$S^aL^a \equiv {}^3P$ and $Q(SL, S^aL^a) = 0$ for nitrogen.

Generally, a partial wave describing the scattering can be written in an asymptotic form proportional to

$$\begin{aligned} r^{-1}k_i^{-1/2}[&\delta_{ii'}\sin(k_ir - \tfrac{1}{2}\pi l_i + \tau_i) \\ &+ \rho_{ii'}\cos(k_ir - \tfrac{1}{2}\pi l_i + \tau_i)],\end{aligned} \tag{8}$$

where i specifies the channel $k_iSL\,l_i\,S^TL^T$ and phases τ_i may be arbitrary. The matrix $\underline{\rho}$ characterizes the scattering and, for each value of S^T, L^T, and parity, it is related to the reactance matrix $\underline{R}$ by

$$\underline{R} = [\sin\tau + (\cos\tau)\underline{\rho}][\cos\tau - (\sin\tau)\underline{\rho}]^{-1},$$

where $\sin\tau$ and $\cos\tau$ represent diagonal matrices.

The asymptotic form of our approximate wave function (4) is proportional to

$$r^{-1}k_i^{-1/2}\sin(k_ir - \tfrac{1}{2}\pi l_i + \eta_i),$$

and η_i depends on the cutoff parameter r_d in the potential (2) or (3). With the choice $\tau_i = \eta_i$, the approximate matrix $\underline{\rho}^t$ describing the scattering is

$$\underline{\rho}^t = 0. \tag{9}$$

Our procedure is to find the "best" form of F_{kl}

by determining the parameter r_d and consequently the phase τ_i for each channel so that, for small variations of r_d,

$$\delta[\rho^t_{ii} - 2\mathcal{L}(SL\, l_i l_i\, S^T L^T)] = 0, \tag{10}$$

while τ_i is not varied. Equation (10) is equivalent to

$$\delta[\eta_i - 2\mathcal{L}] = 0,$$

and from this condition we find r_d and τ_i.

With such F_{kl} in conjunction with (9), the improved approximation to the $\underline{\rho}$ matrix is

$$\rho_{ii'} = -2\mathcal{L}(SL\, l_i l_{i'}\, S^T L^T). \tag{11}$$

The cross sections are calculated from the transition matrix $\underline{T}$, given by

$$\underline{T} = -2i\underline{R}(1 - i\underline{R})^{-1}.$$

For the scattering on the ground states, we have three channels associated with a given $S^T L^T$ for oxygen and one channel for nitrogen.

III. RESULTS AND DISCUSSION

In the calculation of elastic scattering by oxygen and nitrogen in their ground states, we have used Clementi[3] wave functions and dipole polarizabilities α_d obtained by Stevens and Billingsley[4] (0.69 Å^3 for O I and 1.01 Å^3 for N I).

The variation of $\eta - 2\mathcal{L}(SL\, ll\, S^T L^T)$ with the cutoff parameter r_d in the potential (2) is shown in Fig. 1 for oxygen, for partial waves with $l = 0$, $L^T = 1$ at the energy 10 eV. The phase shift η monotonically increases with decreasing r_d, while the expressions $\eta - 2\mathcal{L}$ reach maxima at such values of r_d that the quantity $|2\mathcal{L}|$ is small compared with unity and generally much smaller than the corresponding value calculated without any effect of a polarization potential, (i.e., for $r_d \to \infty$). Partial waves with $l = 1$ and 2 show similar behavior, but in some cases the stationary values of $\eta - 2\mathcal{L}$ correspond to very large r_d, i.e., to the absence of V_p. For $l = 2$, the maxima of $\eta - 2\mathcal{L}$ are less pronounced, and for $l = 3$ the effect of polarization potential is barely noticeable. We have therefore ignored V_p in (1) for all $l > 3$. At energies higher than 50 eV, even the lowest partial waves are not affected by the inclusion of V_p into (1).

For oxygen, we have also calculated $\eta - 2\mathcal{L}$ with the form of V_p given by (3). The effect of different forms of V_p at small r on the stationary values of $\eta - 2\mathcal{L}$ and consequently on the cross sections was found negligible.

There is some uncertainty as to which value of the polarizability α_d should be adopted in (2) or (3). Several values have been reported in the literature.[5] However, our calculations for O I show that the stationary values of $\eta - 2\mathcal{L}$ are only slightly sensitive to α_d. The effect of increasing α_d from 0.69 Å^3 (our adopted value[4]) to 0.77 Å^3 (experimental value[6]) is to change the maxima of $\eta - 2\mathcal{L}$ by less than 0.01, and the resulting change in the cross sections may be considered negligible.

A difficulty arises in the case of oxygen for the matrix element (7) with $l = 1$, $S^T = \frac{1}{2}$, $L^T = 1$, and in the case of nitrogen for $l = 1$, $S^T = 1$, $L^T = 1$, because

$$E'(1s^2\, 2s^2\, 2p^{q+1}\, S^a L^a) - E'(1s^2\, 2s^2\, 2p^q\, SL) - \tfrac{1}{2}k^2 = 0$$

for $\frac{1}{2}k^2 = 0.1529$ (4.16 eV) in O I and 0.2038 (5.55 eV) in N I. As a consequence, the variational correction to the matrix element (11) for energies below 10 eV is not small compared to unity. This suggests that the representation of the trial wave function by (4) in this energy region is not adequate and that the contribution obtained from this element to the cross section is not correct. Under these circumstances, we believe that a more reliable value of the cross section is obtained if we ignore the atomic term in (4), i.e., if we set $c = 0$ and consequently omit the second term in (7).

Results of calculations are given in Table I. Columns labeled (a) and (b) compare cross sections obtained by the method described above, without and with the atomic term in Eq. (4), respectively. In oxygen, the effect of the atomic term is much less pronounced than in nitrogen, despite the singularity of the matrix element (7) at 4.16 eV. In nitrogen, the inclusion of the atomic term in (4) results in a broad shape resonance with the maximum of ~$34.4\pi a_0^2$ at 2.5 eV. Even if we cannot

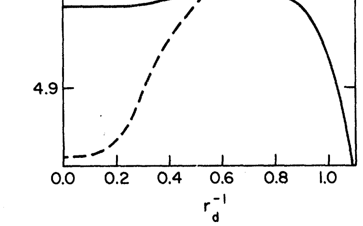

FIG. 1. Full curves: quantity $\eta - 2\mathcal{L}$ calculated for oxygen at 10 eV for two values of S^T and for $l = 0$, as a function of r_d (a.u.) in the polarization potential (2). Dashed curve: corresponding s-wave phase shift η (rad).

TABLE I. Total elastic cross sections (πa_0^2) for scattering from ground states of oxygen and nitrogen.

	Oxygen				Nitrogen			
E (eV)	(a)	(b)	(c)	(d)	(a)	(b)	(c)	(d)
1	8.83	9.55	10.0		12.5	15.7	14.1	
2	9.09	11.0	10.2		13.0	28.5	14.5	
5	9.58	12.1	10.6	16.3	13.5	19.7	14.6	18.6
10	9.16	9.95	9.80	19.9	12.1	14.6	12.6	19.4
20	7.50	7.63	7.60	10.3	9.13	9.45	9.04	10.0
45	4.95	4.96	4.89	4.42	5.40	5.41	5.37	4.51
100	2.96	2.96	2.96	2.46	3.09	3.09	3.09	2.66
500	1.02	1.02	1.02	0.97	1.04	1.04	1.04	1.00

[a] With polarization potential and without atomic term in Eq. (4).

[b] With polarization potential and with atomic term.

[c] Without polarization potential and without atomic term.

[d] Scattering by a static potential.

place much reliability on the cross sections in columns (b) for reasons given above, it is interesting to note that a similar resonance for the elastic scattering on nitrogen was found by Henry *et al.*[7] and by Thompson[8] near 1 eV, by Hunt and Moiseiwitsch[9] at 0.23 eV, and at least an indication of a resonance by Ormonde *et al.*[10] (see Fig. 3). Recently, Burke *et al.*[19] obtained the value 0.062 eV for the position of this resonance. In our model of scattering, the resonance is caused entirely by the inclusion of the potential V_p into Eq. (1). We did not investigate in detail possible improvements in the formulation of the DW approximation in this region, since our main concern was in energies above 10 eV, where the importance of the atomic term rapidly decreases.

The columns labeled (c) in Table I represent cross sections calculated without polarization potential and without the atomic term in Eq. (4); columns (d) show results of scattering by a central potential field which corresponds to the solution of (1) with $V_p = 0$, $\mu_{1s} = \mu_{2s} = \mu_{2p} = 0$, and with $\mathfrak{L}(SL\,ll'\,S^TL^T) = 0$. Cross sections given in columns (d) are identical with values of Wedde and Strand.[11]

A comparison of columns (a) and (c) shows that the effect of the polarization potential is to decrease the cross sections for energies below 20 eV. However, as we took into account only the influence of V_p on the colliding electron and ignored any distortion of the target wave functions, the effect is rather small. A reference to Figs. 2 and 3 will show that below 10 eV and especially below 5

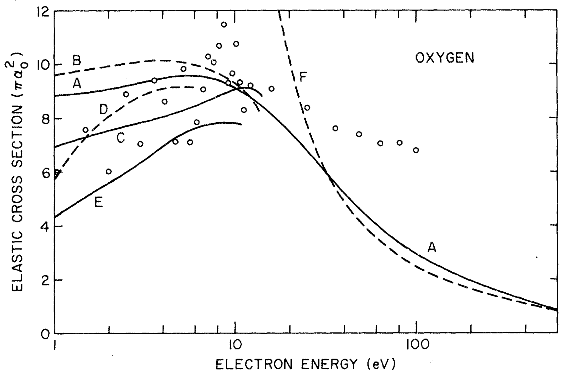

FIG. 2. Elastic cross section for scattering on the ground state of oxygen. Curve A, present result [Col. (a) of Table I]; B, Saraph (Ref. 1), single configuration target (also Henry *et al.*, Ref. 7); C, Saraph (Ref. 1), multiconfiguration target; D, Rountree *et al.*, (Ref. 15); E, Thomas and Nesbet (Ref. 13) (with inelastic contributions); F, Wedde and Strand (Ref. 11) [also Col. (d) of Table I]. Circles—measurements by Sunshine *et al.* (Ref. 16).

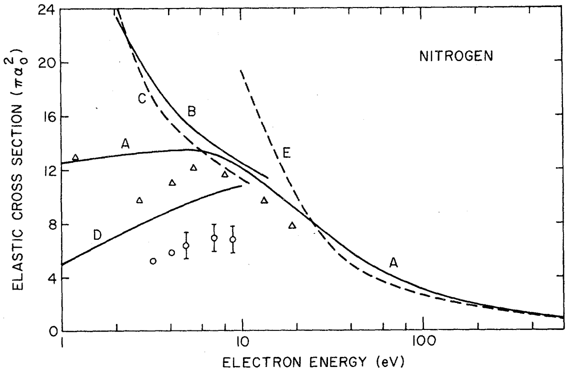

FIG. 3. Elastic cross section for scattering on the ground state of nitrogen. Curve A, present result [Col. (a) of Table I]; B, Henry *et al.* (Ref. 7) (with inelastic contributions); C, Thompson (Ref. 8); D, Henry (Ref. 17); E, Wedde and Strand (Ref. 11) [Col. (d) of Table I]. Triangles—Ormonde *et al.* (Ref. 10); circles—measurements by Neynaber *et al.* (Ref. 18) (only values with highest weight are shown).

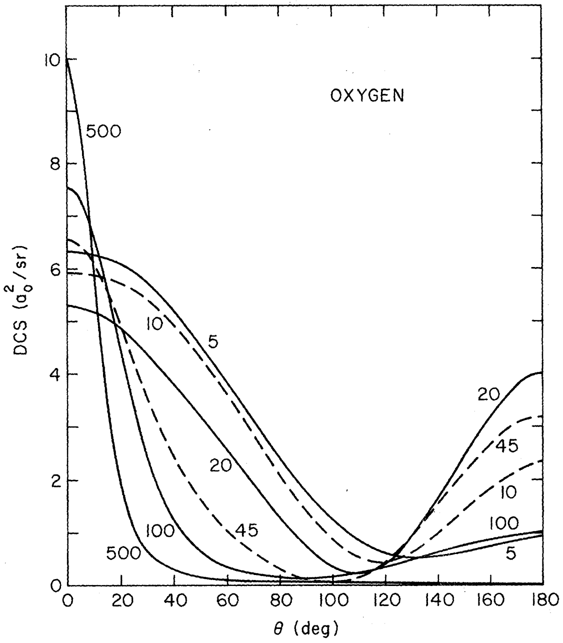

FIG. 4. Differential cross section for elastic scattering on the ground state of oxygen. Labels represent energies in eV.

eV there is a substantial discrepancy between the DW approximation and other methods which use more complicated models for scattering.

Columns (c) and (d) of Table I indicate that the exchange effects decrease the cross sections below 30 eV and increase them for higher energies. At 100 eV, the exchange still contributes ~20% to the elastic cross section. The relative importance of polarization and exchange effects for different energies shown in Table I is in general agreement with results of Thompson.[8]

A comparison of the present results from columns (a) of Table I, which we consider most reliable, with other methods and with experimental data is displayed in Figs. 2 and 3. The discrepancy between the theoretical results and experimental data for nitrogen at low energies was discussed by Ormonde *et al.*[10] Above 20 eV, high measured cross sections for oxygen are probably caused by unresolved inelastic contributions, as suggested by Wedde and Strand.[11]

Differential elastic cross sections obtained from calculations with the potential (2) and without the atomic term are shown in Figs. 4 and 5. They correspond to the total cross sections of columns (a) in Table I. Ratios of the forward to backward scattering, defined by the angles 20–88° and 92–160°, are compared in Table II for oxygen with experimental values of Dehmel *et al.*[12] and theoretical results of Thomas and Nesbet.[13] A comparison of the differential cross sections from Fig. 4 with the results obtained for oxygen by Thomas and Nesbet[13] and by Kutcher *et al.*[14] at energies of 5 and 10 eV shows differences mainly for scattering angles less than 60°. The present approximation predicts higher cross sections for the small-angle scattering in this energy region. Above 45 eV, the general character of the differential cross sections given in Figs. 4 and 5 agrees with results of Wedde and Strand.[11]

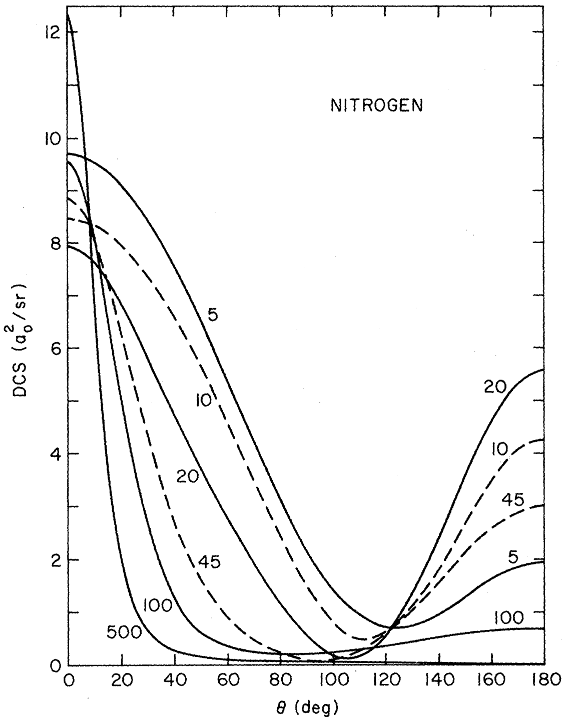

FIG. 5. Differential cross section for elastic scattering on the ground state of nitrogen. Labels represent energies in eV.

Table I and Figs. 2 and 3 lead to the following conclusions: In the present problem, the DW approximation and values shown in column (a) of Table I appear to be accurate within 15% for energies above 10 eV, with improving accuracy at higher energies. The inclusion of a polarization potential improves the results even below this energy, and the effect of this potential can be seen up to 20 eV. Short-range exchange interactions are im-

TABLE II. Ratio of forward to backward elastic scattering by oxygen.

E (eV)	5	10	20
Present result	4.7	4.3	2.9
Dehmel *et al.*, Ref. 12 (expt.)	5.0	3.0	1.6
Thomas and Nesbet, Ref. 13.	3.5	3.7	

portant for energies below 30 eV, but at 100 eV they still contribute as much as 20% to the cross section derived from the potential theory using a central potential.

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