

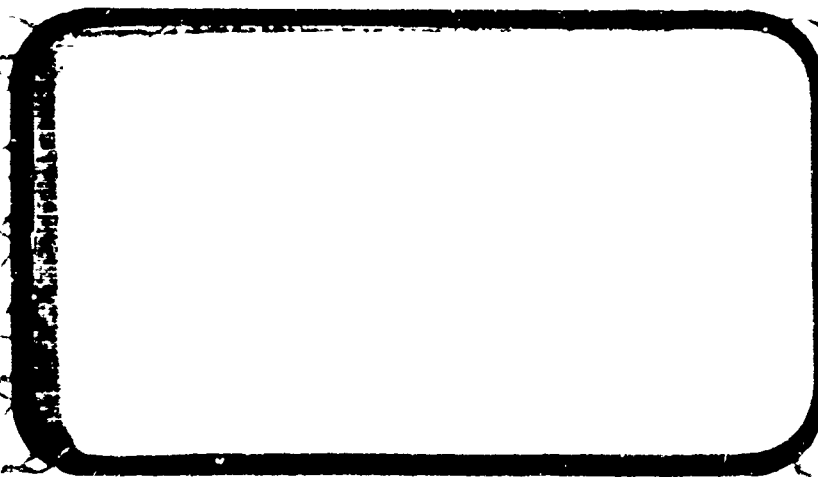
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THE MOMENTUM TRANSFER CROSS SECTION OF ATOMIC NITROGEN
AND ATOMIC OXYGEN FOR LOW ENERGY ELECTRONS

PART I

GM-TR-37

Lawrence Baylor Robinson

ABSTRACT

In this report, an attempt is made to calculate the momentum transfer cross section of atomic nitrogen and atomic oxygen for electrons, especially in the low energy region. This report will consist of four parts. Part I is an introduction to the problem with some preliminary results on nitrogen. Part II will consist of the WBKJ solutions for nitrogen and oxygen with a "zeroth approximation" to the nitrogen and oxygen molecules. Part III will consist of numerical solutions of the (scattering) differential equation, attempts will be made to include the polarization effects of the incoming electrons on the atomic systems. In Part IV, the Born approximation will be made for the high energy range.

1. INTRODUCTION

An understanding of the various processes occurring in the upper atmosphere involves a knowledge of the momentum transfer cross section of atomic nitrogen and atomic oxygen for low energy electrons. Two estimates of the oxygen scattering cross section have been given;¹ evidently none is available for nitrogen. The momentum transfer cross section (sometimes called the diffusion cross section) is given by²

$$Q_d = \frac{2\pi}{4k^2} \int_0^\pi \left| \sum_{\ell=0}^{\infty} (2\ell+1)(e^{2i\delta_\ell} - 1) P_\ell(\cos\theta) \right|^2 (1 - \cos\theta) \sin\theta d\theta$$

$$= \frac{2\pi}{4k^2} \int_{-1}^1 \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} A_m A_n^* P_m(x) P_n(x) (1-x) dx, \quad (1)$$

where $A_j = (2j+1)e^{2i\delta_j}$ and $k^2 = 2mE/\hbar^2$. In Eq. (1), δ_ℓ is the ℓ th order phase shift. The equation may be rewritten as

$$Q_d = Q_o - \frac{2\pi}{4k^2} \sum \sum 2A_{mn} x_{mn}, \quad (2)$$

where

$$Q_o = \sum_{\ell=0}^{\infty} (2\ell+1) \sin^2 \delta_\ell,$$

$$A_{mn} = (A_m A_n^* + A_m^* A_n), \quad (3)$$

$$x_{mn} = \int_{-1}^1 P_m(x) P_n(x) x dx.$$

¹ R. D. Bates and H. S. W. Massey, Proc. Roy. Soc. (London), 192A, 1 (1947).
S. K. Mitra, The Upper Atmosphere, 2nd Edition, The Asiatic Society, Calcutta (1952), p. 260.

² H. S. W. Massey and E. H. S. Burhop, Electronic and Ionic Impact Phenomena, Oxford University Press, London (1952), p. 15.

One may think of the momentum transfer cross section as the elastic scattering cross section plus a correction term. When the scattering is essentially isotropic, these two cross sections differ very little. A matrix representation of x_{mn} (m is the row and n , the column) is

$$x_{mn} = \begin{pmatrix} 0 & 2/3 & 0 & 0 & \vdots \\ 2/3 & 0 & 4/15 & 0 & \vdots \\ 0 & 4/15 & 0 & 6/35 & \vdots \\ 0 & 0 & 6/35 & 0 & \vdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} \quad (4)$$

A convenient representation for A_{mn} is

$$A_{mn} = (2m+1)(2n+1) \left[2 \sin^2 \delta_m - \{ \cos 2\delta_m - \cos 2(\delta_m - \delta_n) \} \right]. \quad (5)$$

The essential part of the problem is the calculation of the phase shifts.

A somewhat detailed description of the method used in obtaining cross sections is given so that the reader will be able to evaluate the range of validity and applicability of the results. The over-all method is to consider the electrons as being scattered from a central field potential. Central field approximations are provided by the statistical atom (Thomas - Fermi) and self-consistent (Hartree - Fock) field. Results for low atomic number (Z) atoms with the statistical field are in general not trustworthy. This is especially so in regard to exceptional atoms like the alkali metals or rare gases. In the calculations given in this report, attempts have been made to include polarization effects.

The Thomas - Fermi potential (c.g.s. electrostatic units) is given by

$$V(x') = - \frac{Z e^2}{b_0 x'} \Phi(x'), \quad (6)$$

where $b_0 = 0.885 Z^{-1/3} a_0$; a_0 is the radius of the first Bohr orbit in

the hydrogen atom and $x' = r/b_o$. One tabulation of the function $\Phi(x)$ is that of Bush and Cardwell.³ The self-consistent field potential is given by⁴

$$V(x) = -\frac{Z\epsilon^2}{a_o x} + \frac{4\pi a_o^2}{M} \left[\frac{1}{x} \int_0^x \left[q_{1s} \{P_{1s}(t)\}^2 + q_{2s} \{P_{2s}(t)\}^2 + q_{2p} \{P_{2p}(t)\}^2 \right] dt \right. \\ \left. + \int_x^\infty \left[q_{1s} \{P_{1s}(t)\}^2 + q_{2s} \{P_{2s}(t)\}^2 + q_{2p} \{P_{2p}(t)\}^2 \right] \frac{dt}{t} \right]. \quad (7)$$

In Eq. (7), the q 's refer to the number of electrons having a given wave function. The P_{1s} , P_{2s} , and P_{2p} are the Hartree-Fock one-electron wave functions for the $1s$, $2s$, and $2p$ electrons in nitrogen⁵ and oxygen⁶ atoms. The functions corresponding only to the ground states, 4S and 3P , respectively, are considered.

$$M = \frac{4\pi a_o^3}{Z\epsilon^2} \int_0^\infty \left[q_{1s} \{P_{1s}(t)\}^2 + q_{2s} \{P_{2s}(t)\}^2 + q_{2p} \{P_{2p}(t)\}^2 \right] dt, \quad (8)$$

and x (or t) = r/a_o . Equation (7) exhibits the potential at a distance x from the origin as being made up of contributions from regions inside and outside x .

An attempt is made to take into account the induced polarization between incoming electron and atom by including a polarization potential which has the following asymptotic form:

$$V_p(x) = -a/x^4. \quad (9)$$

³ V. Bush and S. H. Cardwell, Phys. Rev. 38, 1898 (1931).

⁴ D. R. Hartree, Reports on Progress in Physics 11, 113 (1946-47). Eqs. (20) and (24).

⁵ D. R. Hartree and W. H. Hartree, Proc. Roy. Soc. (London), 193A, 299 (1948).

⁶ D. R. Hartree and B. Swinles, Phil. Trans. Roy. Soc. 238A, 229 (1939).

The manner in which the magnitude of a is estimated is discussed later.

The differential equation from which the cross sections will be determined is that which governs the radial part of the Schroedinger wave function for an incident electron on a central field atom

$$\frac{d^2 U_\ell}{dr^2} + \frac{2}{r} \frac{dU_\ell}{dr} + \left[\frac{2m}{\hbar^2} (E - V(r)) - \frac{\ell(\ell+1)}{r^2} \right] U_\ell = 0. \quad (10)$$

If, instead, one uses $P_\ell = r U_\ell$, the equation is

$$\frac{d^2 P_\ell}{dr^2} + \left[\frac{2m}{\hbar^2} (E - V(r)) - \frac{\ell(\ell+1)}{r^2} \right] P_\ell = 0. \quad (11)$$

The WKBJ solutions⁷ of Eq. (11) in the presence and absence of the scattering potential, yield the following expression for the phase shifts:

$$\begin{aligned} \delta_\ell = & \int_{x_2}^{\infty} \left[(ka_0)^2 - \frac{2mV(x)}{\hbar^2} a_0^2 - \frac{(\ell+1/2)^2}{x^2} \right]^{1/2} dx \\ & - \int_{x_1}^{\infty} \left[(ka_0)^2 - \frac{(\ell+1/2)^2}{x^2} \right]^{1/2} dx, \end{aligned} \quad (12)$$

where x_1 and x_2 are the zeros of the respective integrands. Numerical integrations have been provided by the Computer Systems Division.

⁷ e.g., P. M. Morse and H. Feshbach, Methods of Theoretical Physics, Part II, McGraw-Hill Book Co., New York (1953) pp. 1101-1103.

II. ATOMIC NITROGEN

Preliminary results have been obtained for atomic nitrogen. Table I gives δ_ℓ and $\sigma_\ell = \left[4/(ka_0)^2\right](2\ell+1)\sin^2\delta_\ell$ (in units of πa_0^2) as a function of ka_0 (Mitra's K). The results are not reliable enough to warrant their proposal as an authentic cross section. Errors have come about because of mistakes of the writer. Detailed checkings and recheckings of the procedure have made it so that these errors have now been eliminated and reliable results for the WKBJ solutions for the scattering of electrons by unmodified Hartree potentials should be forthcoming shortly. The same qualitative behavior as reported here is expected.

Table I. Phase Shifts for Electron-Nitrogen Scattering

ka_0	ℓ	δ_ℓ	$\sigma_\ell (\pi a_0^2)$	$\sigma (\pi a_0^2)$
0.25	0	7.29	45.8	45.8
	1	0.002	--	
0.50	0	6.80	3.91	42.7
	1	4.26	38.8	
	2	0.006	--	
0.75	0	6.38	0.069	16.8
	1	4.21	16.4	
	2	0.10	0.4	
	3	0.007	--	
1.00	0	6.02	0.26	30.0
	1	4.06	7.55	
	2	1.36	19.1	
	3	0.046	0.06	
	4	0.007	--	
1.50	0	5.44	0.99	12.2
	1	3.72	1.59	
	2	1.81	8.38	
	3	0.309	1.16	
	4	0.074	0.09	

The results given here suggest that the cross section for atomic nitrogen is about the same order of magnitude as that given by Mitra for oxygen. These results indicate a Ramsauer-Townsend effect. A difference between our results and Mitra's is that our curve tends toward a finite value of the cross section in the low energy range whereas Mitra's does not. Another important result is the strong angular dependence of the scattering, especially as the energy is increased. This means that it is a poor approximation to use the scattering cross section as the diffusion cross section.

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