Theoretical Elastic Collision Frequency between Electrons and Neutral Atoms in a Cesium Plasma*

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(Received April 24, 1961; revised manuscript received May 7, 1962)

The elastic scattering cross sections and momentum transfer cross sections for the collisions of low-energy electrons with atomic cesium have been calculated by the method of phase shifts. The scattering potential, used in the Schrödinger equation, is constructed from one-electron-type wave functions with appropriate screening constants. In addition to the potential arising because of the atomic electrons, a polarization potential is also used; the effect of exchange is considered only indirectly. This preliminary analysis reproduces the shape of the cross section vs energy curves as reported in some experiments but does not give detailed agreement. The theoretical cross sections are averaged over a Boltzmann distribution of electronic energies in the temperature range from 1000 to 10 000°K. Averaged values of the collision (for momentum transfer) frequency between electrons and cesium atoms are also calculated. Results are presented both in graphical and tabular form.

I. INTRODUCTION

SOME transport properties of a cesium plasma are required for an analysis of the performance of a so-called plasma thermocouple. The performance of such a thermocouple is under active investigation at many places in connection with the problem of the direct conversion of heat into electricity. In order to estimate the over-all efficiency of such a device, some estimate of the resistance of the cesium plasma (to the motion of the electrons) is required. The losses to the plasma come about as a result of essentially two mechanisms: (a) the collective interactions of the charged particles, and (b) the collisions of electrons with neutral atoms. In this report, the latter mechanism is discussed; the collective interactions have been extensively studied. In some ranges of temperature and pressure, collisions between electrons and neutral atoms affect the electron distribution function (in the Boltzmann transport equation) to a greater extent than do collisions of the collective type. It is well known that the expression for collision frequency depends on the form of the Boltzmann equation. A simple form of collision frequency is used here.

Among the basic transport parameters required in the investigation of the collisional loss mechanism are the elastic-scattering cross section, the momentum-transfer cross section, and the collision frequency. The elastic-scattering cross section, Q_0, for cesium, as a function of energy, is not known experimentally in the region below 1 eV. Only fragmentary data exist. It is believed that the first detailed theoretical investigation of such cross sections is given in this report.

The elastic-scattering cross section is given by

$$Q_0 = \int_{\theta=0}^{\pi} \int_{\phi=0}^{2\pi} \frac{d\sigma}{d\Omega} \sin\theta d\theta d\phi, \tag{1}$$

where $d\sigma/d\Omega$ is the differential cross section for scatter-

ing the electron into the solid angle $d\Omega = \sin\theta d\theta d\phi$. The values of Q_0 for cesium are calculated in this report. The units of the cross sections are in atomic units, or $a_0^2 = 0.2800 \times 10^{-16}$ cm². The units of energy ϵ are electron volts.

The momentum transfer cross section, Q_M, is given by

$$Q_M = \int_0^{\pi} \int_0^{2\pi} \frac{d\sigma}{d\Omega} (1-\cos\theta) \sin\theta d\theta d\phi. \tag{2}$$

Both Eqs. (1) and (2) result in the familiar phase shift form for the cross section. A value of Q_M for cesium is also calculated.

The collision frequency ν between electrons and neutral atoms is given by

$$\nu = NQ_0 v, \tag{3}$$

where N is the number of neutral atoms per unit volume and v is the electron speed. The collision frequency for momentum transfer ν_M is the parameter which is significant in analyzing the cesium diode. The momentum transfer collision frequency is given by

$$\nu_M = NQ_M v$$

$$= Nv \int_0^{\pi} \int_0^{2\pi} \frac{d\sigma}{d\Omega} (1-\cos\theta) \sin\theta d\theta d\phi. \tag{4}$$

The cross sections as a function of electron energy ϵ are averaged over a Boltzmann distribution, according to the following equations:

$$\bar{Q}_0 = \frac{2}{\pi^{1/2}} \frac{1}{\epsilon_0^{3/2}} \int_0^{\infty} e^{-\epsilon/\epsilon_0} \epsilon^{1/2} Q_0(\epsilon) d\epsilon, \tag{5}$$

$$\bar{Q}_M = \frac{2}{\pi^{1/2}} \frac{1}{\epsilon_0^{3/2}} \int_0^{\infty} e^{-\epsilon/\epsilon_0} \epsilon^{1/2} Q_M(\epsilon) d\epsilon, \tag{6}$$

$$\bar{\nu}_M = \frac{2}{\pi^{1/2}} \frac{1}{\epsilon_0^{3/2}} \left(\frac{2}{M}\right)^{1/2} \int_0^{\infty} e^{-\epsilon/\epsilon_0} \epsilon Q_M(\epsilon) d\epsilon. \tag{7}$$

TABLE I. Parameters for scattering potential for cesium.

i	Z_i	K_i	μ_i	G_i
1	2	109.40	1	U_1
2	8	50.85	2	U_2
3	8	29.167	3	U_3
4	10	22.567	3	U_3
5	8	14.730	3.7	U_4
6	10	8.5676	3.7	U_4
7	8	4.825	4	U_5
8	1	1.0476	4.2	U_6

In Eqs. (5), (6), and (7), $\epsilon_0 = kT$. The averaged collision frequency is given per neutral atom and has units of $cm^3\ sec^{-1}$.

II. THE SCATTERING EQUATION

The cross sections Q_0 and Q_M, for cesium are calculated as outlined elsewhere.[1] Evidently, the Hartree-Fock functions have not been calculated for cesium and it is well known that the Thomas-Fermi model does not describe the alkali atoms too well. Hence, the cesium atom was represented as a Slater orbital type. In this approximation to the mathematical representation of an atom, each electron in the ground state is characterized by a wave function of the form

$$\psi_{\mu_i,l,m} = R_{\mu_i}(r)Y_l^m(\theta,\phi),\qquad (8)$$

where

$$R_{\mu_i} = (K_i)^{\mu_i+1/2}[a_0^3\Gamma(2\mu_i+1)]^{-1/2}e^{-K_ix/2}.\qquad (9)$$

In the equations above, μ_i is an effective principal quantum number, a_0 is the Bohr radius, $\Gamma(2\mu_i+1)$ is the gamma function, and $x=r/a_0$. $K_i=2(Z-S_i)/\mu_i$, where S_i is an appropriate screening constant. The details of the assignment of these parameters are discussed by this writer in reference 1, and numerical values are given in Table III in that report.

The potential which is used in the scattering equation is (in the present formulation)

$$V(x) = -\frac{\epsilon^2}{a_0}\left[\frac{Z}{x} - \sum_{i=1}^{N}\frac{Z_iK_i}{\Gamma(2\mu_i+1)}G_i(K_ix)\right],\qquad (10)$$

where Z_i is the number of electrons in the ith group and N is the total number of groups in the atom. The functions $G_i(K_ix)$ are, with $K_ix=t$, universal functions of t, and are written as[1]

$$U_i(t) = \frac{1}{t}\int_0^t e^{-u}u^{2\mu_i}du + \int_t^\infty e^{-u}u^{2\mu_i-1}du.\qquad (11)$$

Numerical values of the functions $U_i(t)$ are given in Table I in reference 1 and the other parameters for Eq. (10) are given in Table I of this article. In order to obtain values of $U_i(t)$ for arguments which exceed the table, one may use

$$U_i(t) = \Gamma(2\mu_i+1)/t,\quad t\ge t_m,\qquad (12)$$

where t_m is the largest value of t for which $U_i(t)$ is listed.

Experience has shown that the static atom potential alone is (in general) insufficient to provide agreement between theory and experiment. The effects of polarization and exchange must be included. These effects are usually included in the analysis by the addition of a polarization potential to the potential given by Eq. (10). This polarization potential, $V_p(x)$ has the form

$$V_p(x) = -\frac{\epsilon^2}{2a_0}\frac{\alpha}{(x_p^2+x^2)^2}.\qquad (13)$$

In Eq. (8), α is the polarization parameter and x_p is the so-called screening distance. Both α and x_p are in atomic units. The inclusion of exchange, in some cases, has been effected by a slight alteration of the strength and range of the polarization.[2] The manner in which α and x_p are selected is discussed in Sec. III.

In this present analysis, the scattering cross sections have been obtained with and without the inclusion of the polarization potential in the scattering equation. The scattering equations, without polarization and with polarization, respectively, are

$$\frac{d^2y_l}{dx^2}+\left\{(ka_0)^2+2\left[\frac{Z}{x}-\sum_{i=1}^{N}\frac{Z_iK_i}{(2\mu_i+1)}G_i(K_ix)\right]-\frac{l(l+1)}{x^2}\right\}y_l=0,\qquad (14)$$

and

$$\frac{d^2y_l}{dx^2}+\left\{(ka_0)^2+2\left[\frac{Z}{x}-\sum_{i=1}^{N}\frac{Z_iK_i}{(2\mu_i+1)}G_i(K_ix)+\frac{1}{2}\frac{\alpha}{(x_p^2+x^2)^2}\right]-\frac{l(l+1)}{x^2}\right\}y_l=0.\qquad (15)$$

The scattering equation, with the potential attributed entirely to polarization, is

$$\frac{d^2y_l}{dx^2}+\left[(ka_0)^2+\frac{\alpha}{(x_p^2+x^2)^2}-\frac{l(l+1)}{x^2}\right]y_l=0.\qquad (16)$$

Such an equation has also been considered in this report in order to determine the extent to which the polarization potential alone can give satisfactory results.

This report contains the results of the *first steps* in an investigation which hopes to provide a guide as to the magnitudes of the cross sections to be expected in

[1] L. B. Robinson, Aerospace Corporation Report No. TDR-594(1203-01)TR-1, in which cross sections are given in terms of the phase shift representation (unpublished).

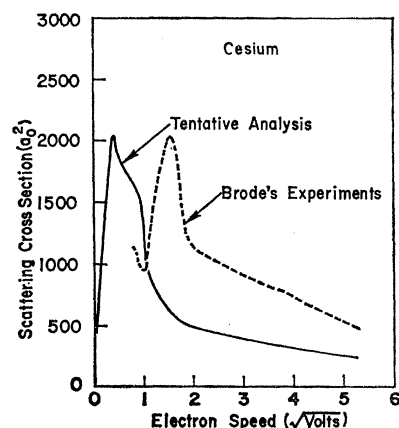[2] M. M. Klein and K. A. Brueckner, Phys. Rev. 111, 1115 (1958).

FIG. 1. Comparison of experimental and theoretical results.

such low energy ranges. In this present analysis, the emphasis has been placed on direct scattering, the situation in which the incoming electron always becomes the scattered electron. The possibility of an exchange between incident electron and one of the electrons of the target atoms is considered only indirectly. A subsequent investigation will consider the effect of taking exchange into account more directly.

III. RESULTS

Because the potential used for the alkali atoms extends over a much greater range than that of the noble gas atoms, or atomic oxygen, more phase shifts are required in this present analysis than have been used before. For the larger values of $(ka_0)^2$, as many as 15 values of l were used. The decision in this regard was to use no more than 15 values of δ_l in the calculation of the cross sections. When no polarization potential was used, the integration of the differential equation, Eq. (14), was carried out to $x=25$ where the phase shifts were calculated. The potential vanishes for cesium before this point. When the polarization potential was included, the integration was carried out to $x=100$ where the phase shifts were calculated. At $x=100$, the polarization potential is negligible and going out further made only minor differences as will be seen later.

Calculations were made in which no polarization potential is used. Over most of the energy range, except in the vicinity of zero energy, the calculated cross sections were about an order of magnitude smaller than the experimental cross sections of Brode.[3] Experience with such cross-section calculations has shown that the potential from the atomic electrons, without a polarization potential, rarely gives agreement between theory and experiment.

Equation (15) was integrated to give the phase shifts, with several values of α and x_p. The results of the calculation are quite sensitive to these parameters (more sensitive to α than to x_p). In practically all cases, the same shape of cross section vs energy curve

was obtained. The procedure used in obtaining the polarization potential is not completely satisfactory, but it seems to be the best that is available for the present situation. The parameter α is taken to be the polarizability of the alkali atom. The assignment of the polarization radius (r_p) is more difficult, even conceptually. For the purpose of this present analysis, the polarization radius was taken to be just the "radius" of the atom. Since the concept of atomic radius is not a unique concept, the preceding sentence will be clarified further in the next paragraph.

Three methods were used in fixing the atomic radius: (a) calculation from the wave functions, (b) assignment from gas kinetic values, and (c) arbitrary assignments. Because of the form of the screening-constants-type wave functions, the kth power of the radius of electron orbital designated by μ_i is[4]

$$\bar{r}_{\mu_i}{}^k = \frac{\displaystyle\int_0^\infty r^{k+2}|R_{\mu_i}|^2 dr}{\displaystyle\int_0^\infty r^2|R_{\mu_i}|^2 dr}$$

$$= \left[\frac{\mu_i}{2(Z-S_i)}\right]^k \left[\prod_{m=1}^k (2\mu_i+m)\right]a_0{}^k. \quad (17)$$

With $k=2$, the numerical value of $r_p{}^2$, given by,

$$r_p{}^2 = \sum_{i=1}^N \bar{r}_{\mu_i}{}^2, \quad (18)$$

turned out to be, almost exactly, $(\alpha/2)^{2/3}$, where α is the most up-to-data available polarizability.[5] This is true also for rubidium. Hence, the polarization potential could be written as

$$V_p = \frac{1}{2} \frac{\alpha}{[(\alpha/2)^{2/3}+x_p{}^2]^2}. \quad (19)$$

It is recalled that $x=r/a_0$. The preceding considerations convert the polarization potential from a two-parameter into a one-parameter function.

The polarizability α of cesium,[5] which was used in obtaining the cross sections given in Fig. 1, is $\alpha=36 \times 10^{-24}$ cm^3, which in atomic units is 243. The polarization distance x_p was taken as $(\alpha/2)^{1/3}$, which gives $x_p{}^2=24.5$. The cross sections are also shown in Fig. 1. These results are typical of all those in which a polarization potential was used. The agreement between theory and Brode's experiments is of the same type as is accepted for agreement between theory and experi-

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TABLE II. Effect of final point in solution of scattering equation on values of cross sections.

	$x_l = 100.00$			$x_l = 150.00$		
l	δ_l	$\Sigma_l \sigma_l$	Q_M	δ_l	$\Sigma_l \sigma_l$	Q_M
0	0.0335854	14.1693		0.0343922	14.8580	
1	3.07360	188.167		3.07477	182.921	
2	6.28975	190.876	270.274	6.29208	187.894	275.070

TABLE III. Averaged cross sections and collision frequency.

	Cesium		
$T(°K)$	$\bar{Q}_0 \ (a_0{}^2)$	$\bar{Q}_M \ (a_0{}^2)$	$10^6 \bar{\nu}_M$
1000	1588	1419	0.7665
2000	1709	1223	0.8538
3000	1685	1070	0.8812
4000	1619	969.0	0.9200
5000	1542	896.6	0.9487
6000	1466	841.1	0.9719
7000	1393	795.9	0.9892
8000	1327	757.6	1.0013
9000	1267	723.9	1.0085
10000	1212	693.9	1.0121

ment in the case of sodium.[6] A similar calculation for rubidium did not give as good agreement; also not as much time was taken as with cesium.

In addition to the results given in Fig. 1, calculations were made with[7] $\alpha = 42 \times 10^{-24}$ cm³; the corresponding value of $x_p{}^2$ is 27.5. Calculations were made with values of x_p obtained from listed values of the radius of cesium and values were also arbitrarily assigned. No better agreement between theory and Brode's experiment was obtained than is shown in Fig. 1.

One might try to improve the results by using potential functions determined from Hartree-Fock functions, which are more characteristic of specific atoms. Such functions must first be calculated. Experience with phase-shift determinations would suggest that the improvement by the use of the unmodified Hartree-Fock functions will not be dramatic. One cannot predict the effect of the inclusion of a polarization potential (with the Hartree-Fock potential) in a direct way. It seems as if the next step, in addition to that of obtaining new experimental data (especially in the low-energy region), is to take exchange scattering into account in a direct way.

Since the inclusion of the polarization potential made such a difference in the results, a study was made to see if the polarization potential by itself would be sufficient to account for the results of Fig. 1. The solutions of Eq. (11) showed that this is not the case. Without the atomic electrons, the results were in disagreement with Fig. 1 everywhere except at zero energy. This agreement here is perhaps accidental, since the signs of the scattering length are opposite for the two cases.

When the polarization potential is not included, a suitable point at which to stop the integration of the scattering equation is quite evident in that the potential vanishes for some value of x, as can be seen from Eq. (10). The polarization potential does not vanish, except at $x = \infty$. It was observed that integrating out to $x = 75$ gave results which differed by an order of magnitude from those obtained at $x = 100$, whereas going out to 150 made only a difference of 2 to 3% at most from results obtained at $x = 100$. Table II shows the effect of the end point of the integration. In this case $\alpha = 42 \times 10^{-24}$ cm² and $x_p{}^2 = 16.0$ (arbitrarily assigned) atomic units.

The cross sections shown in Fig. 1 were averaged

over a Boltzmann distribution according to Eqs. (5), (6), and (7) for values of the temperature ranging from $T = 1000°K$ to $T = 10\ 000°K$. The results are shown in Table III. Also $\bar{Q}_M$ (the average value of the momentum transfer cross section) and $\bar{\nu}_M$ (the average collision frequency) are given in Fig. 2. In order to convert the cross sections to cm², the ordinates must be multiplied by $0.2800 \times 10^{-16} \times 10^2$. For example, $\bar{Q}_M$ at $5000°K$ is $9 \times 0.2800 \times 10^{-14} = 2.52 \times 10^{-14}$ cm². At $3000°K$, the collision frequency is approximately 9×10^{-7} cm³ sec⁻¹ per atom. In order to obtain the collision frequency for an actual situation, one must multiply the values given here by the number of neutral cesium atoms per cm³. It is quite likely that these tentative results will not prove to agree with experiments (yet to be performed) in detail; the present aim is to provide a guide for planning in the absence of experimental information. This writer is also studying methods of taking exchange into account more directly.

It is also of interest to compare this theoretical estimate of electron collision frequency with experiment. Measurements of electron mobilities in the positive column by Boeckner and Mohler[8] yield an average electron collision frequency of 1.6×10^{-6} cm³ sec⁻¹ per atom which is independent of electron energy
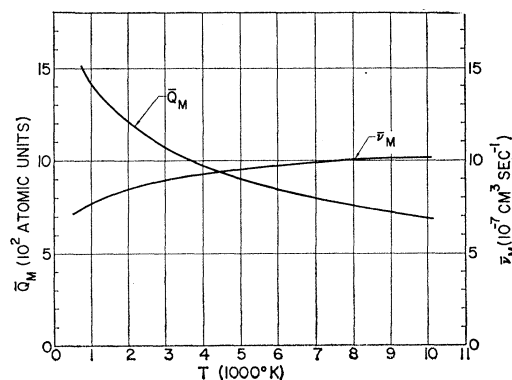

FIG. 2. Theoretical collision frequency and momentum transfer cross section for cesium.

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in the range between 0.2 and 0.4 eV. The original data given in the above reference have been corrected by Phelps[9] on the basis of additional experiments of Mohler.[10] The value of 1.6×10^{-6} cm³ sec⁻¹ per atom is the result of Phelps' correction. It is of interest to note that this value is almost in exact agreement with the value which is obtained in this article if the total scattering cross section, rather than the momentum transfer cross section (see Table III) is used in calculation of collision frequency.

Preliminary experiments of G. J. Mullaney at General Electric Company indicate values of the cross section much lower than those reported here. Corresponding experiments of C. L. Chen, M. Rather, and colleagues

at the University of Illinois suggest cross sections much higher than those reported here (for the energy range less than 1 eV). More experiments are required before this cesium cross section can be known with reliability. Of course, the tentative theoretical cross section given in Fig. 1 should never be used as a basis for comparison with experiment without mentioning that the analysis is tentative and that the limitations of the analysis are fully realized. *It is usually easier to get agreement between theory and experiment, once the experimental result is known.*

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Investigations of Paramagnetic Neutron Scattering from Chromium

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Neutron diffraction investigations on Cr⁵² indicate that localized atomic magnetic moments do not exist in metallic chromium above the Néel temperature. Therefore, the moments which exist in the antiferromagnetic structure are presumably induced during the ordering process.

INTRODUCTION

THE early neutron diffraction experiments on chromium metal[1] showed it to be antiferromagnetic at low temperatures. Since this time numerous investigations have been performed in an attempt to gain a better understanding of the magnetic behavior of this metal and, hence, also of the 3d metals in general.

It was shown by Corliss, Hastings, and Weiss[2] in experiments on a single crystal of chromium that there exists a long-range modulation of the antiferromagnetic moment distribution. This was first interpreted in terms of an antiphase domain structure, but it is now recognized that other possible magnetic structures are a spiral arrangement of the moments[3,4] and an ordered moment arrangement similar to that found in erbium,[5] in which the magnitudes of the magnetic moments are sinusoidally modulated. Investigations by Shirane and

Takei[6] strongly indicate that the magnetic structure belongs to the latter class.

The antiferromagnetic transition in chromium also has a somewhat unusual behavior. Recent neutron diffraction investigations[2,7–9] have shown that single-crystal chromium samples have a Néel temperature near 310°K, whereas this transition occurs near 450°K in certain powdered samples. Since careful studies have revealed anomalies in the electrical resistivity,[10] Hall effect,[11] magnetic susceptibility,[12] and specific heat[13] near the lower temperature, this value is believed to correspond to the antiferromagnetic transition in pure strain-free chromium. It can only be surmised that the higher magnetic ordering temperature in some chrom-

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