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Elastic Scattering of Slow Electrons by Cesium Atoms*

PHILIP M. STONE† AND JOHN R. REITZ‡
Los Alamos Scientific Laboratory, University of California, Los Alamos, New Mexico

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The elastic scattering cross section for the scattering of slow electrons by cesium atoms has been calculated for incident electron energies ranging from 0.0005 to 0.13 Ry. The model used is an adiabatic one which includes exchange. By means of a partial-wave expansion the problem is reduced to the solution of an integrodifferential equation for each partial wave. The results of the calculation show rough agreement with low-energy plasma resistivity experiments and with collision-time measurements, but do not support the microwave experiments of Chen and Raether. The results of the calculation are quite sensitive to the inclusion of exchange and to the form of the polarization potential; arguments are presented to show that optimum parameters of an adiabatic model have been used in the present calculation.

I. INTRODUCTION

CURRENT interest in thermionic converters using ionized cesium vapor has stimulated renewed interest in the transport properties of a cesium plasma. In particular, a number of recent experimental studies[1-4] have been directed toward a determination of the electron-neutral cesium atom cross section, a quantity which controls the electrical resistivity of weakly ionized plasmas. Except for the results of Chen and Raether[4] these experiments, together with earlier measurements by Boeckner and Mohler,[5] give a coherent but rough picture of the scattering cross section at electron energies below 0.4 eV. The discrepancy between these experiments and those of Chen and Raether is yet to be resolved. The scattering cross section of cesium for electron energies above 0.6 eV is known from the early work of Brode.[6]

The purpose of the present investigation is to provide a quantum-mechanical (phase shift) calculation of the elastic-scattering cross section. Although there have been extensive calculations of electron-hydrogen scattering,[7] there has been only a limited amount of work directed toward the scattering of slow electrons by heavier atoms. We must mention, however, a recent calculation by Robinson[8] of the elastic scattering of electrons by cesium atoms, which calculation was extended to extremely small incident velocities. Robinson's work unfortunately suffers from several defects: (1) He did not have self-consistent wave functions for cesium, so he approximated by using Slater-type orbitals; (2) he did not include exchange; and (3) although his "polarization potential" was correct asymptotically, it was adjusted more or less arbitrarily at intermediate radii. We have found that the results of the calculation are quite sensitive to the effective scattering potential presented by the atomic system, and furthermore that the inclusion of exchange completely alters the low-energy cross section.

The model we have chosen to investigate is the *adiabatic model*, so-called because the atomic system is allowed to polarize in response to the instantaneous position of the bombarding electron. For the low-incident energies in which we are primarily interested, the collision time is long compared to characteristic atomic periods, and the atomic wave function can readily adjust to the perturbing influence of the incident electron; this, of course, is just the basis for the adiabatic model. The model, thus, introduces a "polarization potential" in a natural way.

We have investigated the adiabatic model both with and without exchange effects. In the no-exchange case the problem can be reduced (by expansion in partial waves) to the solution of an ordinary differential equation, whereas in the exchange case the problem reduces to the solution of an integrodifferential equation. Although these equations can be solved by straightforward numerical methods, the procedure here is somewhat more complicated than in the case of electron-hydrogen scattering. In the first place, many more particle waves are required, a fact already apparent from Robinson's work.[8] Secondly, an iterative solution to the integrodifferential equation, which appears to work so well in the hydrogen-atom problem,[9] was found unsatisfactory here, particularly for the lower order partial waves, so that a noniterative solution was required. Finally, since the polarizability of the cesium atom is much larger than that of hydrogen, the "polar-

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[†] Present address: Sperry Rand Research Center, North Road, Sudbury, Massachusetts.

[‡] Permanent address: Case Institute of Technology, Cleveland, Ohio.

[1] G. J. Mullaney and N. R. Dibelius, Am. Rocket Soc. **31**, 1575 (1961).

[2] D. Roehling, Symposium on Thermionic Power Conversion, Colorado Springs, May, 1962. [J. Energy Conversion (to be published).]

[3] R. K. Flavin and R. G. Meyerand, Jr., Symposium on Thermionic Power Conversion, Colorado Springs, May, 1962. [J. Energy Conversion (to be published).] The cross sections reported in this paper are too low by a factor of 2π [R. K. Flavin (private communication)].

[4] C. L. Chen and M. Raether, Phys. Rev. **128**, 2679 (1962).

[5] C. Boeckner and F. L. Mohler, J. Res. Natl. Bur. Std. **10**, 357 (1933).

[6] Robert B. Brode, Phys. Rev. **34**, 673 (1929).

[7] See P. G. Burke and K. Smith, Rev. Mod. Phys. **34**, 458 (1962), and references quoted there.

[8] L. B. Robinson, Phys. Rev. **127**, 2076 (1962).

[9] P. G. Burke and H. M. Schey, Phys. Rev. **126**, 147 (1962).

ization potential" must be introduced into the problem with considerable case.

II. FORMULATION OF THE PROBLEM

The scattering of slow electrons by cesium atoms is essentially a two-electron problem (the bound electron outside the closed shell and the bombarding electron). The Schrödinger equation for the system may be written as[10]

$$\left[\nabla_1^2+\nabla_2^2+E+\frac{2Z(r_1)}{r_1}+\frac{2Z(r_2)}{r_2}-\frac{2}{r_{12}}\right]\Psi(\mathbf{r}_1,\mathbf{r}_2)=0, \quad (1)$$

where $\mathbf{r}_1$ and $\mathbf{r}_2$ are position vectors to electrons 1 and 2, respectively, and $r_{12}=|\mathbf{r}_1-\mathbf{r}_2|$. $Z(r)$ is the effective charge of the cesium ion core at position r. We were fortunate in having a numerical tabulation of $Z(r)$, as well as ground-state and excited-state wave functions of the cesium atom, from earlier work by one of the authors.[11] In effect, $Z(r)/r$ is a Prokovief potential, a modification of the Hartree potential of the Cs^+ ion, which has been adjusted empirically to reproduce a large number of the term values in the spectrum of atomic cesium; it is described fully in Ref. 11.

In order to solve Eq. (1) in a practical way, some approximation must be introduced. One of the simpler approximations which has yielded satisfactory results for electron-hydrogen scattering is the *static-exchange model* in which Ψ is approximated by $\psi_0(\mathbf{r}_1)F(\mathbf{r}_2)\pm\psi_0(\mathbf{r}_2)F(\mathbf{r}_1)$, where ψ_0 is the ground-state wave function of the atomic electron. Polarization effects can be effectively included by adding an appropriate polarization potential term to the integrodifferential equation for F. This was essentially the approximation which we wanted to use, the only difficulty being that because polarization effects are much more important in cesium than in hydrogen, it is important that the polarization potential showing up in the equation for F be approximately correct at all radii. In order to introduce this potential in a natural way, we go over to the *adiabatic model*:

$$\Psi(\mathbf{r}_1,\mathbf{r}_2)=\psi_0'(\mathbf{r}_1)F(\mathbf{r}_2), \quad \text{(adiabatic, no exchange)} \quad (2a)$$

$$\Psi(\mathbf{r}_1,\mathbf{r}_2)=\psi_0'(\mathbf{r}_1)F(\mathbf{r}_2)\pm\psi_0(\mathbf{r}_2)F(\mathbf{r}_1), \quad \text{(adiabatic with exchange)} \quad (2b)$$

where ψ_0 is the ground-state wave function of the atomic system, and ψ_0' is a perturbed ground-state function, perturbed (adiabatically) by the presence of the second electron.

The plus sign in Eq. (2b) refers to the symmetric (singlet) state of the two electrons, and the minus sign to the antisymmetric (triplet) state. The use of ψ_0 instead of ψ_0' in the $\pm$ term is a defect of the model since it destroys the symmetry of the wave function, but the consistent use of ψ_0' would result in considerable complication: The radial equations resulting from the partial wave expansion would not decouple. We felt justified in using Eq. (2b) as it stands since the major purpose of substituting ψ_0' for ψ_0 in the static model is to introduce the polarization potential in a natural way. Errors caused by the omission of the neglected terms in (2b) are discussed in Sec. V.

The perturbed ground-state wave function ψ_0' may be expressed as[12]

$$\psi_0'(\mathbf{r}_1)=\psi_0(\mathbf{r}_1)+\sum_n{}'\beta_n(\mathbf{r}_2)\psi_n(\mathbf{r}_1), \quad (3)$$

where the summation is over the complete set of atomic functions. For the problem under consideration, we have found it sufficient to express ψ_0' as

$$\psi_0'(\mathbf{r}_1)=\psi_0(\mathbf{r}_1)+\beta_1(r_2)\psi_1(\mathbf{r}_1), \quad (4)$$

where ψ_1 is a particular excited state wave function, namely, the $6p$ function. Therefore, we shall limit the discussion here to equations of the form of Eq. (4). The validity of this approximation and the form of $\beta(r_2)$ will be discussed in the next section.

Equation (2b), with ψ_0' defined by Eq. (4), may now be substituted into the Schrödinger equation, Eq. (1). If this equation is multiplied on the left by ψ_0^* and the result integrated over the coordinates of particle 1, one obtains

$$(\nabla_2^2+k_0^2-V_{00}-v_p)F(\mathbf{r}_2) =\mp\int d\tau_1\,\psi_0^*(\mathbf{r}_1)\left(k_0^2-E_0-\frac{2}{r_{12}}\right)F(\mathbf{r}_1)\psi_0(\mathbf{r}_2), \quad (5)$$

where the upper sign refers to the singlet, and the lower sign to the triplet state. Here $k_0^2\equiv E-E_0$ is the kinetic energy of the incident electron, E_0 being the ground-state energy of the cesium atom, and V_{00} is defined as

$$V_{00}(r_2)=\left\langle\psi_0\left|\frac{2}{r_{12}}-\frac{2Z(r_2)}{r_2}\right|\psi_0\right\rangle. \quad (6)$$

The polarization potential, v_p is defined to be

$$v_p(r_2)=\beta_1(r_2)V_{10}=\beta_1(r_2)\left\langle\psi_0\left|\frac{2}{r_{12}}\right|\psi_1\right\rangle. \quad (7)$$

Equation (5) can be reduced to a radial equation through the use of a partial-wave expansion:

$$F(\mathbf{r}_2)=\sum_l r^{-1}f_l(r)P_l(\cos\theta_2). \quad (8)$$

Both V_{00} and v_p are spherically symmetric, so that

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[10] We use atomic units (a.u.) throughout this paper; i.e., all distances are measured in units of Bohr radii, all energies in Ry. Cross sections will be expressed in units of πa_0^2.

[11] P. M. Stone, Phys. Rev. **127**, 1151 (1962).

[12] See Ref. 7, p. 488.

Eq. (5) becomes

$$f_l''+\left[k_0^2-V_{00}-v_p-\frac{l(l+1)}{r^2}\right]f_l=\pm\phi_0 \times\left[(E_0-k_0^2)\delta_{l0}\int_0^\infty f_0\phi_0 dr+\left\{\frac{2}{(2l+1)}\right\} \times\left\{r^l\int_0^\infty f_l\phi_0 r^{-(l+1)}dr+r^{-(l+1)}\int_0^r f_l\phi_0 r^l dr -r^l\int_0^r f_l\phi_0 r^{-(l+1)}dr\right\}\right], \quad (9)$$

where $r^{-1}\phi_0$ is the normalized radial part of the ground-state wave function ψ_0. The integrodifferential Eq. (9) may be solved in a noniterative fashion by the procedure used by Marriott.[13] We note that Eq. (9) has the form

$$f_l''+\gamma(r)f_l=\pm\xi(r,f_l)\pm r^l\phi_0\times(\text{sum of definite integrals involving } f_l). \quad (10)$$

If we write

$$f_l(r)=g_l(r)+A_l n_l(r), \quad (11)$$

then g_l and n_l satisfy the following differential equations:

$$g_l''+\gamma(r)g_l=\pm\xi(r,g_l), \quad (12a)$$

$$n_l''+\gamma(r)n_l=\pm\xi(r,n_l)\pm r^l\phi_0, \quad (12b)$$

provided

$$A_l=\left\{(E_0-k_0^2)\delta_{l0}\int_0^\infty g_l\phi_0 dr+\left[\frac{2}{(2l+1)}\right] \times\int_0^\infty g_l\phi_0 r^{-(l+1)}dr\right\}\bigg/\left\{1-(E_0-k_0^2)\delta_{l0} \times\int_0^\infty n_l\phi_0 dr-\left[\frac{2}{(2l+1)}\right]\int_0^\infty n_l\phi_0 r^{-(l+1)}dr\right\}. \quad (13)$$

The differential equations, (12a) and (12b), may be solved numerically, A can be calculated, and finally f_l may be calculated by means of Eq. (11).

III. THE POLARIZATION POTENTIAL

The use of Eq. (3) for the perturbed ground-state wave function leads to a polarization potential of the form

$$v_p(\mathbf{r}_2)=\sum_n{}'\beta_n(\mathbf{r}_2)V_{n0}(\mathbf{r}_2). \quad (14)$$

When the bombarding electron is far from the atom, the coefficients β_n may be evaluated from perturbation theory. Thus,

$$\beta_n(\mathbf{r}_2)=-\frac{V_{0n}(\mathbf{r}_2)}{(E_n-E_0)} \quad (15)$$

and

$$v_p=-\sum_n{}'|V_{0n}|^2/(E_n-E_0). \quad (16)$$

Now the ground state of the atom (both cesium and hydrogen) is an s state, so that at very large distances the dominant contribution to the sum in Eq. (16) comes from perturbing p states, and v_p takes the form

$$v_p(r)=-2\alpha/r^4, \quad (17)$$

where α is to be identified with the polarizability of the atom.

Castillejo, Percival, and Seaton[14] have shown that the first excited state ($2p$) contributes 65.8% of the long-range polarization in hydrogen. In cesium the first excited state ($6p$) lies only 0.1036 Ry above the ground state, and we find that this state contributes 92% of the long-range polarization. At closer radii other excited states (particularly the $7s$ and continuum states) become more important, but we find that the $6p$ state is still the most important perturbing state at all important radii ($r>3$ to 4 a.u.). At still closer radii, the potential V_{00} dominates the solution of the differential equation. We have, therefore, been led to consider Eq. (4) as an appropriate choice for the perturbed ground state, ψ_0'. If we measure the polar angle θ_1 [where $\psi_1(\mathbf{r}_1)=\psi_1(r_1,\theta_1,\varphi_1)$] from the axis defined by the instantaneous position of electron 2, we need consider only one of the $6p$ states, namely, that corresponding to $m=0$.

One is tempted to use the perturbation solution for $\beta_1(r_2)$, namely, Eq. (15), at all radii. However, a numerical calculation of V_{10} shows that this is not justified at intermediate radii. We have, therefore, treated Eq. (4) as a trial wave function for $\psi_0'(\mathbf{r}_1)$, with β_1 a variational parameter. In the spirit of the adiabatic approximation,

$$H=H_0(\mathbf{r}_1)+V'(\mathbf{r}_1,\mathbf{r}_2), \quad (18)$$

where

$$H_0=-\nabla_1^2-2Z(r_1)/r_1,$$

$$V'=2/r_{12}-2Z(r_2)/r_2.$$

The total energy is given by

$$E=(1+\beta_1^2)^{-1}[E_0+\beta_1^2E_1+V_{00}+\beta_1^2V_{11}+2\beta_1V_{10}], \quad (19)$$

where V_{00} and V_{10} have been previously defined, and V_{11} is given by

$$V_{11}(r_2)=\langle\psi_1|V'|\psi_1\rangle. \quad (20)$$

If $dE/d\beta$ is set equal to zero, one finds, after some algebra, that $\beta_1(r_2)$ can be obtained from the equation

$$\frac{\beta_1}{(1-\beta_1^2)}=-\frac{V_{10}}{(E_1-E_0+V_{11}-V_{00})}, \quad (21)$$

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[13] R. Marriott, Proc. Phys. Soc. (London) 72, 121 (1958).

[14] L. Castillejo, I. C. Percival, and M. J. Seaton, Proc. Roy. Soc. (London) A254, 259 (1960).

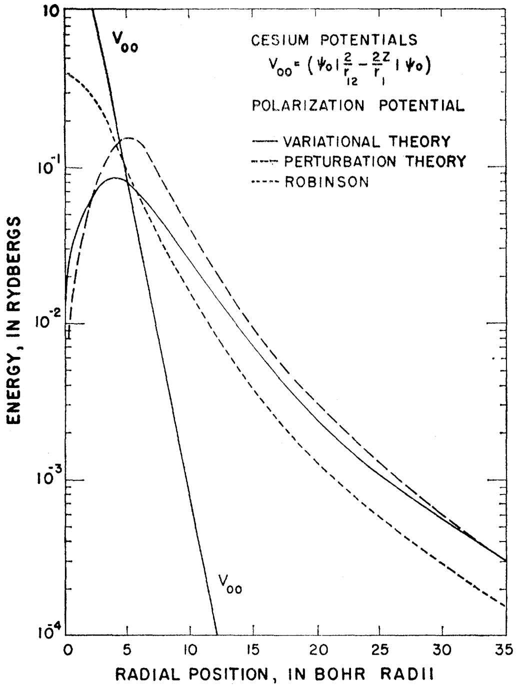

FIG. 1. Potentials for cesium. The negative of the potentials has been plotted; i.e., they are all negative potentials. The polarization potential of Robinson (Ref. 8) is apparently small by a factor of 2 at large radii.

which reduces to the perturbation theory result at large radii (i.e., large r_2).

We have calculated $\beta_1(r_2)$ numerically from Eq. (21) and used the result to calculate the polarization potential according to Eq. (7). Since this gives only 92% of the long-range polarization, we have scaled up the potential by a constant factor, so that asymptotically v_p is given by Eq. (17) with α the experimentally observed[15] polarizability (243 a.u.) of the atom. The polarization potential so calculated is plotted in Fig.1 along with the perturbation-theory result.

In addition to the polarization of the valence electron, there is another polarization effect which is not contained within the two-electron picture. This is polarization of the Cs ion core, and this leads to a polarization potential of the form $-2\alpha_c/r^4$. The experimental value[16] of α_c is 8.22 a.u., which is small compared to the atomic value. Thus, core polarization does not appear to be particularly important, but even so we have effectively included it by scaling our result to agree with the experimental polarization of the atom (valence electron plus core) at large distances.

IV. NUMERICAL PROCEDURE

The differential equations describing the elastic scattering problem were integrated numerically on an IBM-704 computer. The initial phase of the problem consisted of computing the radial functions ϕ_0 and ϕ_1 from the input data $Z(r)$. Next, the potential integrals, $V_{00}(r_2)$, $V_{10}(r_2)$, and $V_{11}(r_2)$, were computed and stored in the machine.

The solutions to the differential equations (12) for g_l and n_l were started at the origin with a power series development which included terms through r^6. The equations were then integrated forward by the Numerov method,[17] which is an integration scheme accurate to the fifth power of the interval size. The integrations were carried out to $r=40$ at an interval size of $h=0.02$. At this point, A_l [defined by Eq. (13)] was calculated, the function f_l formed, and the integration of f_l continued at an interval size $h=0.2$ to $r=92$. During the last integration the right-hand side of Eq. (9), as well as V_{00}, was set equal to zero, and the polarization potential was accurately approximated by

$$v_p = -486/(r^2+25)^2; \quad r>40. \tag{22}$$

Integrals of the type $\int_0^r q(r')dr'$ appearing in the differential equation were calculated by the trapezoidal rule using the integration mesh h.

At $r=92$ the phase shift δ_l was determined directly from the code. δ_l is defined by the asymptotic form of f_l

$$\begin{aligned} f_l &\to C_1 r j_l(kr) + C_2 r n_l(kr) \\ &\to (1/k)[C_1 \sin(kr - \tfrac{1}{2}l\pi) - C_2 \cos(kr - \tfrac{1}{2}l\pi)] \\ &= (C_3/k) \sin(kr + \delta_l - \tfrac{1}{2}l\pi). \end{aligned} \tag{23}$$

The code determined C_1 and C_2 by comparing the numerical solution at the last two mesh points with the spherical Bessel functions (obtained by a standard subroutine.

A check on the accuracy of the integration procedure was made by turning the integration around at $r=40$ and integrating backwards to the origin. Comparison of the solutions shows that the functions agree to three significant figures. Round-off error propagating through the large number of mesh points of the integration destroyed the remaining digits. An over-all check of the effect of round-off and truncation error was determined by calculating the spherical Bessel functions using our code with all potentials set equal to zero. The resulting phase shifts differed from zero by the order of -0.0005 rad in all cases.

V. THE SCATTERING CROSS SECTION

The elastic-scattering cross section may be calculated once the phase shifts are known. For the case of no

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[15] G. E. Chamberlain and J. C. Zorn, Bull. Am. Phys. Soc. **5**, 241 (1960); J. C. Zorn and P. Fontana, *ibid.* **5**, 242 (1960).

[16] F. S. Ham, in *Solid State Physics*, edited by F. Seitz and D. Turnbull (Academic Press Inc., New York, 1955), Vol. 1, p. 176.

[17] B. Numerov, Publ. Observ. Astrophys. Cent. Russie (Moscow) **11** (1923); Monthly Notices Roy. Astron. Soc. **84**, 592 (1924). See also, G. W. Pratt, Phys. Rev. **88**, 1217 (1952).

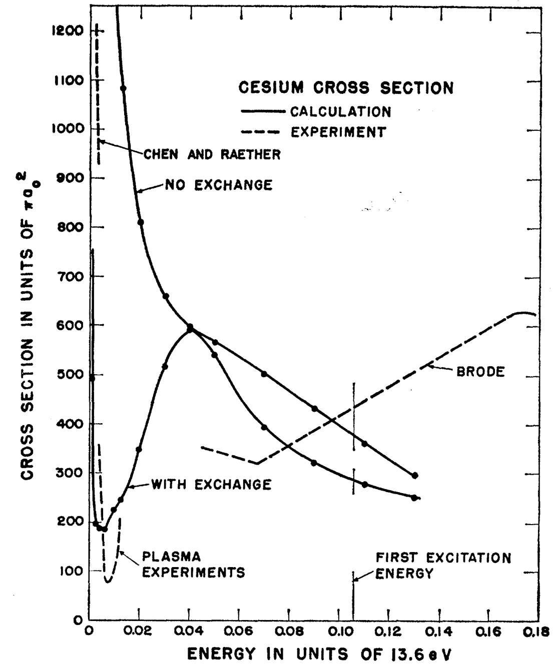

FIG. 2. Elastic-scattering cross section for slow electrons on cesium atoms. Brode's (Ref. 6) experiment measures the total scattering cross section so that the rise of his values above the first excitation energy is due to inelastic collisions. The part marked "plasma experiments" is qualitative only. For details of this region, see Fig. 4. The data of Chen and Raether (Ref. 4) are also shown.

exchange, the cross section (in units of πa_0^2, with a_0=Bohr radius) is given by the usual phase-shift expression,

$$\sigma=\left(\frac{4}{k^2}\right)\sum_l (2l+1)\sin^2\delta_l^0. \tag{24}$$

Here the superscript 0 refers to the no-exchange case. When exchange is included, the cross section may be written

$$\sigma=\tfrac{1}{4}\sigma^{+}+\tfrac{3}{4}\sigma^{-}, \tag{25}$$

where σ^+ and σ^- are calculated from expressions of type (24) with δ_l^0 replaced by δ_l^+ or δ_l^-, respectively. The superscript (+) refers to the singlet, and the (−) to a triplet state of the system.

Phase shifts and cross sections were calculated for incident electron energies (k_0^2) ranging from 0.0005 to 0.13. Enough partial waves were included to insure convergence of (24) and (25); at the highest energies we required seven partial waves. The numerical values of the phase shifts are tabulated in Table I, and the calculated cross sections are plotted in Fig. 2 along with some experimental results. It is apparent from the figure that the inclusion of exchange has a drastic effect on the cross section at low energies. The no-exchange case does not agree with experiment, but the calculation which includes exchange, while it by no means gives good agreement, does reproduce the trend of the experi-

TABLE I. Calculated phase shifts.[a]

Phase shifts—No exchange (δ_l^0)

k^2	$l=0$	$l=1$	$l=2$
0.001	9.523	3.323	0.014
0.003	9.349	3.898	0.046
0.005	9.220	4.410	0.077
0.007	9.103	4.642	0.110
0.010	8.954	4.773	0.152
0.013	8.837	4.824	0.205
0.020	8.613	4.826	0.311
0.030	8.367	4.773	0.472
0.040	8.184	4.713	0.638
0.050	8.027	4.654	0.800
0.070	7.783	4.549	1.128
0.090	7.613	4.452	1.435
0.110	7.428	4.370	1.695
0.130	7.343	4.291	1.892

Phase shifts—With exchange
Symmetric case (δ_l^+)

k^2	$l=0$	$l=1$	$l=2$
0.001	9.248	3.241	0.014
0.003	8.996	3.400	0.046
0.005	8.822	3.531	0.078
0.007	8.673	3.599	0.105
0.010	8.493	3.655	0.147
0.013	8.353	3.691	0.183
0.020	8.095	3.699	0.274
0.030	7.818	3.660	0.371
0.040	7.621	3.621	0.446
0.050	7.456	3.579	0.508
0.070	7.221	3.531	0.629
0.090	7.045	3.505	0.755
0.110	6.916	3.505	0.933
0.130	6.810	3.512	1.155

Phase shifts—With exchange
Antisymmetric case (δ_l^-)

k^2	$l=0$	$l=1$	$l=2$
0.001	9.799	6.336	0.017
0.003	9.648	6.330	0.052
0.005	9.524	6.301	0.086
0.007	9.410	6.254	0.104
0.010	9.260	6.156	0.181
0.013	9.146	6.086	0.220
0.020	8.922	5.910	0.428
0.030	8.665	5.708	0.841
0.040	8.471	5.562	1.289
0.050	8.302	5.403	1.675
0.070	8.039	5.177	2.080
0.090	7.821	4.993	2.222
0.110	7.647	4.841	2.314
0.130	7.493	4.712	2.363

Phase shifts for higher l
$\delta_l^0\approx\delta_l^+\approx\delta_l^-$

k^2	$l=3$[b]	$l=4$[b]	$l=5$	$l=6$	$l=7$
0.001	0.005	0.002	0.001	...	...
0.003	0.015	0.006	0.002	...	...
0.005	0.024	0.010	0.004	...	...
0.007	0.034	0.015	0.008	...	...
0.010	0.048	0.021	0.011	...	...
0.013	0.065	0.029	0.015	...	...
0.020	0.099	0.046	0.024	...	...
0.030	0.138	0.062	0.034	...	...
0.040	0.181	0.086	0.049	...	...
0.050	0.217	0.104	0.059	...	...
0.070	0.285	0.139	0.078	0.048	...
0.090	0.340	0.167	0.095	0.059	0.039
0.110	0.393	0.199	0.115	0.073	0.049
0.130	0.437	0.225	0.131	0.084	0.056

[a] An integral number of π's have been added to the $l=0$ and $l=1$ phase shifts so that the phase shifts decrease with increasing l.

[b] At energies above $k^2=0.04$ the exchange phase shifts begin to differ noticeably from the no-exchange phase shifts. The difference increases linearly so that at $k^2=0.13$ the δ_3^+ and δ_3^- are 14% below and above (respectively) the listed values. Similarly, δ_4^+ and δ_4^- are 2.5% below and above the listed values.

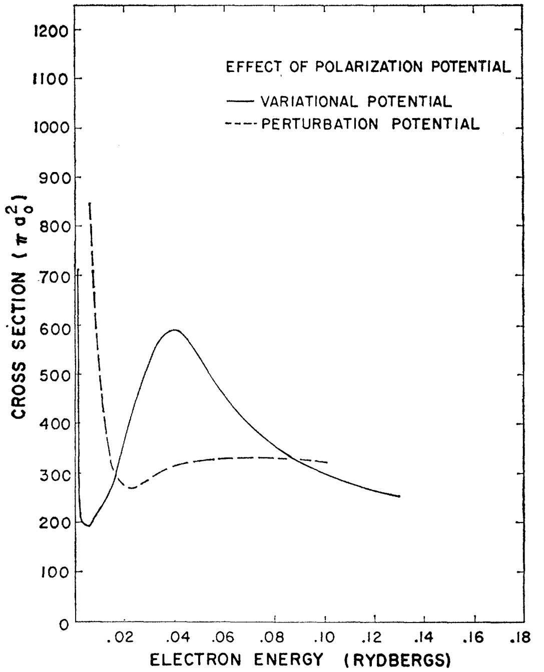

FIG. 3. Effect of polarization potential on calculated elastic-scattering cross section. The polarization potential obtained from perturbation theory gives a cross section with a smaller minimum and no peak at $k^2=0.04$. Both calculations include exchange.

ments (a minimum cross section at about 0.09 eV). At the higher energies (above 0.08) our calculation may be compared with Brode's experimental results. Brode's results are for total cross section and, therefore, include both elastic and inelastic contributions; the peak that Brode found at 0.17, and which drops off at higher energies, is presumably due to inelastic collisions (excitation). Thus, our higher energy results appear to be reasonable. As expected, the effect of exchange becomes less important at the higher energies.

In order to determine how sensitive the results of the calculation are to variations in potential, the polarization potential was varied. As a preliminary check, the no-exchange case was rerun with only 90% of the polarization potential. The cross section showed changes of from 10 to 20%, but the basic form of the cross section versus energy curve was preserved. However, when the shape of the polarization potential was modified, the cross section was altered rather substantially. Our calculation was repeated, both for the exchange and no-exchange case, using the polarization potential as determined from perturbation theory (see Fig. 1). The results with exchange are shown in Fig. 3, where it is seen that a substantially larger polarization potential at intermediate radii has almost completely eliminated the low-energy dip in the cross section. At energies above 0.08, variations in polarization potential have a relatively small effect. Furthermore, as noted, the effect of exchanges becomes less important at high energies, and our calculation appears to extrapolate smoothly into Robinson's high energy results.[8]

An attempt was made to estimate the consequences of using ψ_0 instead of ψ_0' in the $\pm$ term of Ψ, Eq. (2b). When ψ_0' is used, the equation for $F(\mathbf{r}_2)$, Eq. (5), has a second term on the right side, namely,

$$\pm\int d\tau_1\psi_0^*(\mathbf{r}_1)\left(\frac{2}{r_{12}}-\frac{2Z(r_2)}{r_2}\right)\beta_1(\mathbf{r}_1)F(\mathbf{r}_1)\psi_1(\mathbf{r}_2). \quad (26)$$

This term is smaller than the first term because $\beta(r_1)$ is small at large radii where ψ_1 is important, and $\psi_1(\mathbf{r}_2)$ itself is smaller than $\psi_0(\mathbf{r}_2)$ at the critical radii of about 4–10 a.u. A comparison of the two terms by graphical integration—using $F(\mathbf{r}_1)$ as calculated, i.e., without the second term—indicates that the second term is less than 20% of the first. Though this is not negligible, it implies changes in the phase shifts of only a few percent.

A further attempt to determine the effect of this lack of full symmetry in the wave function[18] was made by normalizing the ψ_0' part of Ψ. Thus, calculations were rerun using

$$\Psi(\mathbf{r}_1,\mathbf{r}_2)=\frac{1}{[1+\beta_1^2(\mathbf{r}_1)]^{1/2}}\psi_0'(\mathbf{r}_1)F(\mathbf{r}_2)\pm\psi_0(\mathbf{r}_2)F(\mathbf{r}_1), \quad (27)$$

leading to Eq. (5) with the right side multiplied by $[1+\beta^2(\mathbf{r}_1)]^{1/2}$. This increases the right side by considerably more than the addition of Eq. (26), and so has an exaggerated effect. The result of the calculation was a decrease in the cross section of less than 4% at energies $k^2\leq 0.20$, a decrease of nearly 10% near $k^2=0.05$ and a decrease of less than 5% at higher energies. It is clear, then, that the neglected term gives only a small contribution.

Figure 4 shows our calculated low-energy cross section replotted on a different scale, together with the results of various groups of experimenters. Since plasma resistivity experiments really measure a momentum-transfer cross section, defined by

$$\sigma_M=\int\frac{d\sigma}{d\Omega}(1-\cos\theta)d\Omega, \quad (28)$$

we have calculated the latter quantity from our phase shifts, and this result is also plotted on Fig. 4 for a limited range of energies. Actually, the momentum transfer cross section is not very different from the elastic scattering cross section in this energy range.

Finally, it is perhaps worthwhile to note that the rapid rise of the calculated cross section at low energies

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[18] The choice between Eqs. (2b) and (27) is not clear-cut. Since ψ_0 and ψ_1 are individually normalized, Eq. (27) is the natural consequence of using Eq. (4). On the other hand, Eq. (4) is not really correct at the smaller radii, since there is an appreciable admixture of excited s states. It was felt, at least initially, that the unnormalized ψ_0' is a somewhat better approximation to the correct adiabatic wave functions in the 2–4 Å range, whereas at the larger radii the normalization is not important.

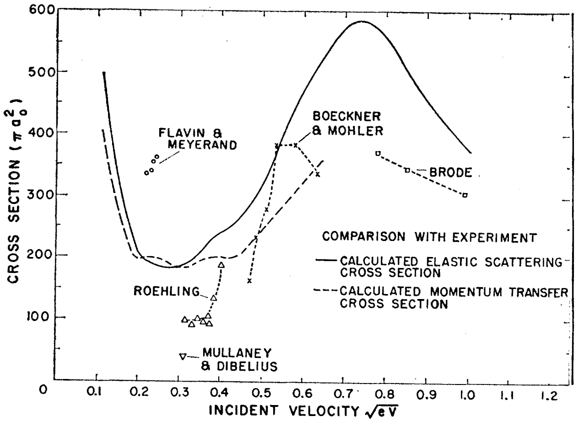

FIG. 4. Comparison with experiment. All except Brode's experiment are momentum-transfer cross sections and are averages over the electron velocity distributions of a plasma. The correct values of Flavin and Meyerand are shown (see Ref. 3). The results of Chen and Raether are not shown on this plot (see Fig. 2).

implies that care is necessary when assigning energies to experimentally obtained cross sections. All the experiments referred to in Fig. 4, except Brode, involve electrons with a distribution of velocities, presumably Maxwellian. Thus, the slower moving electrons may contribute strongly to the over-all results in some experiments, but in others (such as plasma resistivity measurements) electrons with low-scattering cross sections will presumably contribute more heavily.

VI. CONCLUSIONS

The adiabatic model has been extended about as far as is possible. The model predicts an elastic-scattering cross section in rough agreement with most experimental results, although the lowest energy (plasma resistivity) experiments differ by about a factor of 2 from our calculation. Because of the sensitivity of the calculation to the form of the polarization potential, it appears quite possible that a better estimate of this quantity could improve the agreement. One way of improving the polarization potential would be to go over to the close-coupling model[7] in which only terms involving ψ_0 and ψ_1 are retained in the wave function. Here ψ_0 is the ground state, and ψ_1 the first excited p state of the atom. Such a model should be better suited to cesium than to hydrogen; however, the model leads to coupled integrodifferential equations and is about an order of magnitude more difficult than the adiabatic model considered here.

Note added in proof. Equation (17) should read $v_P(r) = -\alpha/r^4$; i.e., the factor of 2 should not be present. Our calculation of the long-range potential is then a calculation of the polarizability giving a value of $\alpha = 66.5 \times 10^{-24}$ cm^3, in complete agreement with the calculation of Sternheimer[19] but considerably greater than experiment.[20] The small up-scaling mentioned near the end of Sec. III is not appropriate but can be considered as including to some extent the effects of higher states and the polarizability of the core. In any case, the phase shifts are not sensitive to this up-scaling and the results are nearly unchanged. The authors are indebted to Dr. Peter Bender and Dr. Thomas F. O'Malley for pointing out this error in the identification of the polarizability.

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