Elastic Scattering of Low-Energy Electrons by the Thomas-Fermi Atom

LAWRENCE BAYLOR ROBINSON
Space Technology Laboratories, Inc., Los Angeles, California
(Received September 28, 1959)

A detailed study has been made of the elastic scattering properties of the Thomas-Fermi atom for low-energy electrons. The scattering lengths have been determined for essentially all atoms in the periodic table within the framework of the Thomas-Fermi approximation. The scattering length is not a monotone function, but rather a periodic (roughly) function of the atomic number of the scattering atom. Both positive and negative scattering lengths are found.

The effect of the sign and magnitude of the scattering length on the shape of the cross section *versus* energy curve is studied. It is observed that atoms with negative scattering lengths have very low cross sections for some energy of the incoming electrons; such is not the case with all atoms having positive scattering lengths.

I. INTRODUCTION

VARIOUS types of schematic central field potentials have been used in investigations of the elastic scattering of low-energy electrons by atoms. One such potential is given by

$$V(r)=Z\epsilon^2[(1/r)-(1/r_0)],\quad r\leqslant r_0 \qquad V(r)=0.\quad r>r_0 \tag{1}$$

In Eq. (1), Z is the atomic number of the target (scattering) atom, ϵ is the electronic charge, and r_0 is a parameter with dimensions of length. Allis and Morse[1] obtained cross sections for a variety of values of the parameters Z and r_0. Another such potential is

$$V(r)=(Z\epsilon^2/r)e^{-2r/r_0}, \tag{2}$$

where the parameters have the same significance as in Eq. (1). Morse[2] investigated scattering properties of this potential for various values of Z and r_0.

This article gives the results of an investigation of the elastic scattering of low-energy electrons with a schematic potential based on the Thomas-Fermi function. An advantage in using the Thomas-Fermi potential is that only one parameter (the atomic number Z of the target atom) is involved. This potential is somewhat realistic in describing collisions with real atoms of large Z; the electronic distribution is derived from a statistical treatment of the atom. Exceptions are to be expected for large atoms like the alkali atoms or small atoms like the noble gas atoms.

II. THE SCATTERING CROSS SECTION AND SCATTERING LENGTH

The scattering cross section σ is given by

$$\sigma=\sum_{l=0}^{\infty}\sigma_l=\sum_{l=0}^{\infty}\frac{4\pi}{k^2}(2l+1)\sin^2\delta_l, \tag{3}$$

where $k^2=2mE/\hbar^2$ and δ_l is the lth order phase shift. E is the kinetic energy of the incoming electrons and m is the electronic mass. The phase shifts, δ_l, are calculated in a well-known manner from the radial part of the Schrödinger equation,

$$\frac{d^2R_l}{dr^2}+\left(\frac{2m}{\hbar^2}[E-V(r)]-\frac{l(l+1)}{r^2}\right)R_l=0. \tag{4}$$

The Thomas-Fermi potential is

$$V(r)=-(Z\epsilon^2/r)\phi(r/b), \tag{5}$$

where Z is the atomic number of the target atom and ϵ is the electronic charge. The constant b is given by

$$b=0.885a_0/Z^{\frac{1}{3}}, \tag{6}$$

where a_0 is the Bohr radius of the lowest orbit in the hydrogen atom. The function $\phi(x)$ is the solution of the equation

$$d^2\phi/dx^2=\phi^{\frac{3}{2}}/x^{\frac{1}{2}}, \tag{7}$$

with boundary conditions $\phi(0)=1$ and $\phi(\infty)=0$. The tabulated values of the function given by Bush and Caldwell[3] were used in the present calculations.

The substitution $x=r/b$ converts Eq. (4) into

$$\frac{d^2y_l}{dx^2}+\left((kb)^2+\frac{2mb}{\hbar^2}\frac{Z\epsilon^2}{x}\phi(x)-\frac{l(l+1)}{x^2}\right)y_l=0. \tag{8}$$

The asymptotic phases were calculated in essentially the same manner as described by this writer in connection with a similar problem.[4] In this present work, Eq. (8) was integrated numerically with the Space Technology Laboratories IBM-704 Electronic Computer.

Zero energy cross sections for the Thomas-Fermi potential have been calculated by this writer before.[5]

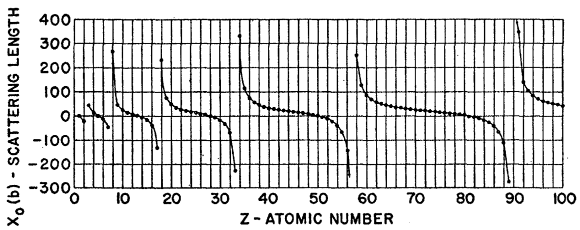

FIG. 1. Scattering length (in units of b) as a function of atomic number.

[1] W. Allis and P. M. Morse, Z. Physik **70**, 567 (1931).
[2] P. M. Morse, Revs. Modern Phys. 4, 557 (1932).
[3] V. Bush and S. H. Caldwell, Phys. Rev. **38**, 1898 (1931).
[4] L. B. Robinson, Phys. Rev. **105**, 922 (1957).
[5] L. B. Robinson, The Ramo-Wooldridge Corporation Report ERL-108, June, 1957 (unpublished).

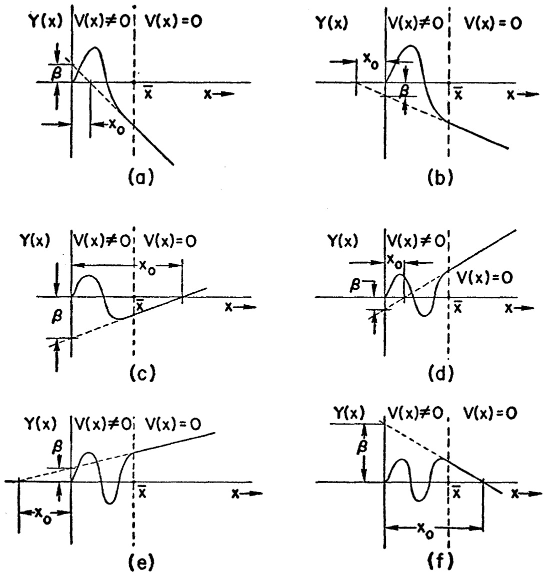

FIG. 2. Wave functions and scattering lengths.

The present work enlarges the scope of the previous work in that energy dependent cross sections have been calculated for several values of Z. The manner in which the zero energy cross section and the scattering length are calculated is discussed in the next paragraph.

The zero energy cross section is calculated as follows: As the energy approaches zero, only the $l=0$ phase shift is different from zero and the cross section is given by

$$\sigma=(4\pi/k^2)\sin^2\delta_0. \tag{9}$$

The wave equations become

$$y''+(2mb/\hbar^2)V(x)y=0, \tag{10}$$

where $V(x)$ is the Thomas-Fermi potential. If $\bar{x}$ is the point where $V(x)$ becomes negligible, outside $\bar{x}$ the solution starts out like a straight line or

$$y=Cx+\beta, \tag{11}$$

where C is the slope and β is the intercept on the y-axis. The intercept on the x-axis, x_0, is the so-called scattering length or extrapolated Fermi intercept. From Eq. (11), it is seen that

$$x_0=-\beta/C, \tag{12}$$

and this determines the value of the zero energy cross section. In order that σ in Eq. (9) be finite, it is required that $\sin^2\delta_0$ approach zero, as k approaches zero. Hence Eq. (9) may be written as

$$\sigma=(4\pi/k^2)\delta_0^2. \tag{13}$$

In the low-energy limit, instead of having a true phase shift as given by

$$y=B\sin(kx+\delta_0), \tag{14}$$

one has

$$y=B(kx+\delta_0),\ \text{approximately}. \tag{15}$$

From Eq. (15), one obtains for the Fermi intercept, i.e., when $y=0$,

$$x_0=-\delta_0/k, \tag{16}$$

or from Eq. (13)

$$\sigma=4\pi x_0^2. \tag{17}$$

The cross section given in Eq. (3) is derived from the following relation,

$$\sigma=\int_0^{4\pi}|f(\theta,\phi)|^2d\Omega, \tag{18}$$

where $f(\theta,\phi)$ is amplitude of the scattered wave. When $f(\theta,\phi)$ is a constant (dimensions of length), it follows that

$$\sigma=4\pi f^2=4\pi x_0^2. \tag{19}$$

One sees that the amplitude of the scattered wave for zero energy incident electrons is an equivalent definition of the scattering length.

III. RESULTS

Equation (8) was first integrated, with $k^2=0$, for values of Z from 1 to 100. The low values of Z are included in order to obtain a more complete picture of the scattering properties of the Thomas-Fermi potential. It is understood that the very low values of Z have no significance as far as a statistical interpretation of atoms is concerned. In line with other results obtainable from this potential, one would expect the theoretical results to conform to experiments for the case of high Z atoms, except possibly for alkali and noble gas atoms which are not described too well by the Thomas-Fermi potential.

The scattering lengths, x_0, are plotted against Z in Fig. 1. The calculations show that x_0 (and hence the zero energy cross section) is not a monotone, but a periodic function of Z. The curve given in Fig. 1 has as many branches as there are periods in the periodic table. The breaks in the curve do not always coincide with the beginning or ending of a period. The values of x_0 for $Z=57$ and 90 are 1.83×10^7 and 3.99×10^7 (in units of b), respectively; these values are too large to show on the graph.

The behavior of the wave function y as a function of x is given in Fig. 2. In each case $\bar{x}$ is the point at which the potential is considered zero; the function y is a straight line for $x>\bar{x}$. In Fig. 2(a), $\beta>0$, $C<0$, $y(\bar{x})<0$, and $x_0>0$. Figure 2(a) shows the behavior of the wave function and scattering lengths for $Z=1$, 10–13 (i.e., all Z including 10 and 13), 39–50. In Fig. 2(b), $\beta<0$, $C<0$, $y(\bar{x})<0$, and $\bar{x}_0<0$, which is the behavior for $Z=2$, 14–17, 51–57. Figure 2(c) shows $\beta<0$, $C>0$, $y(\bar{x})<0$ and $x_0>0$, which is the behavior for $Z=3$, 18–20, 58–64. Figure 2(d) shows $\beta<0$, $C>0$, $y(\bar{x})>0$, and $x_0>0$; this type of curve is obtained for $Z=4$, 5, 21–28, 65–81. Figure 2(e) has $\beta>0$, $C>0$, $y(\bar{x})>0$, and $x_0<0$ as found for $Z=6$, 7, 29–33, 82–89. Figure 2(f) has $\beta>0$, $C<0$, $y(\bar{x})>0$, and $x_0>0$. This type of behavior was found for $Z=8$, 9, 34–38, 90–100.

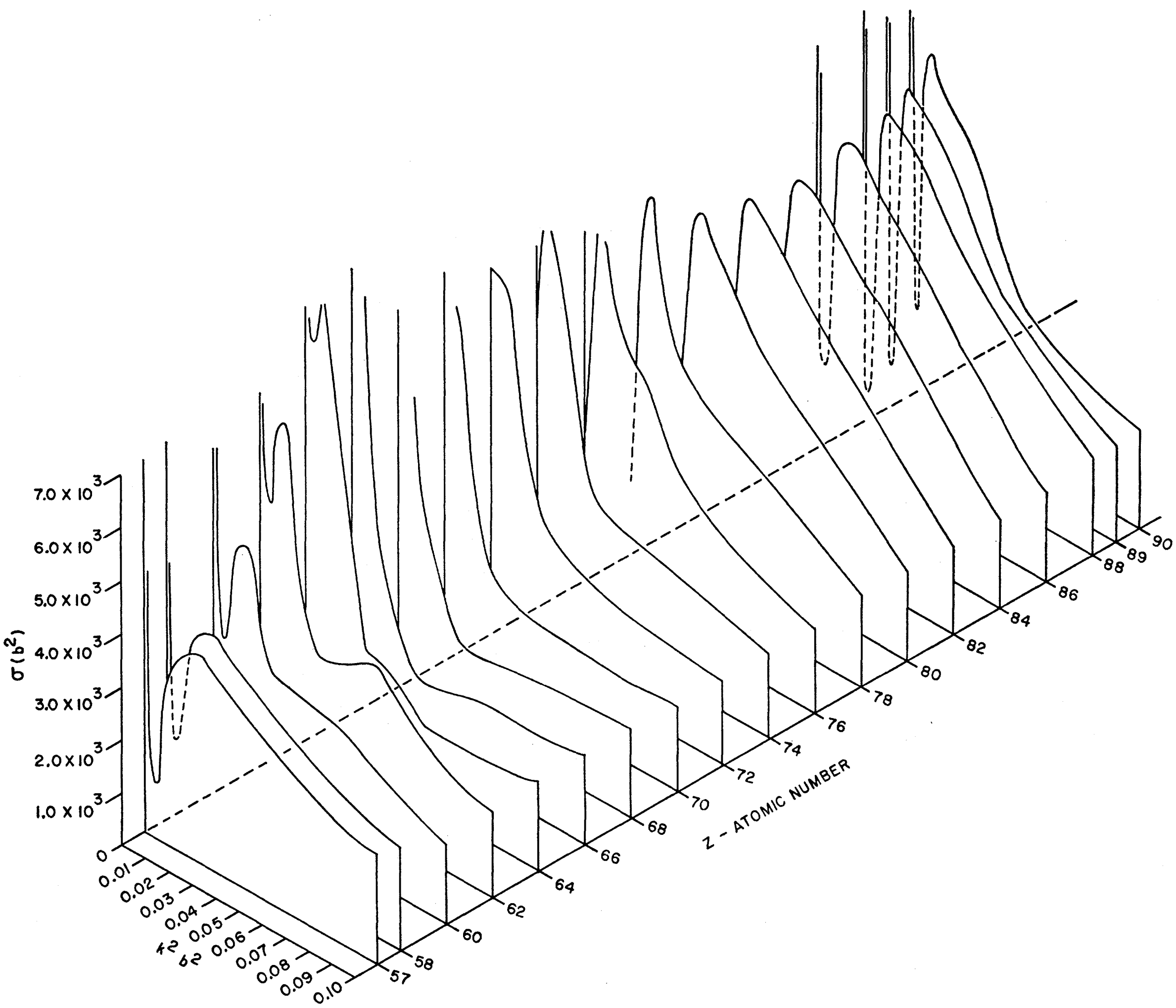

FIG. 3. Cross sections in units of b^2 as a function of $(kb)^2$ and atomic number.

Bound states can exist only for the situations represented by Figs. 2(c) and 2(f).

Since the scattering length is to some extent periodic in some function of Z, this writer believes that a complete study of the effect of scattering length on the shape of the cross-section energy curve can be obtained by studying only one period. The period selected for study was the one beginning with $Z=58$ and ending with $Z=89$. The points $Z=57$ and 90 are also included in the study. The results are given in Fig. 3. The values of $(kb)^2$ range from zero to 0.1 in steps of 0.01. In all cases, both for $k=0$ and $k\neq 0$, the Thomas-Fermi potential was assumed to vanish at $x=\bar{x}=43.48$.

It is interesting to note that the scattering lengths at and near the ends of period display the typical Ramsauer-Townsend effect. As one goes from $Z=57$, 58, and 60 the minimum in the cross-section curve becomes higher and higher and finally disappears at $Z=66$. The zero energy cross section is always finite and is given by Eq. (19). As the (positive) scattering lengths become smaller, the curve bends over more quickly to meet the vertical axis. At $Z=74$ a maximum (without the adjacent minimum) appears; the zero value of the cross section decreases because the scattering lengths have become smaller. At $Z=80$, 81, and 82, the zero energy cross section is practically zero. Following this, the minimum reappears. All negative scattering lengths show a low cross section for some ranges of incident electron energies. There are no negative scattering lengths which give cross section typical of those for the range $Z=66$ to 72. The typical Ramsauer-Townsend effect is characterized by a large negative scattering length or a large positive scattering length such that the wave function is negative when the potential vanishes.

ACKNOWLEDGMENTS

The writer is indebted to Dr. James Riley and Mr. Malcom Perry for assistance with the numerical aspects of the problem.