CLASSICAL CALCULATIONS OF DIFFERENTIAL SCATTERING CROSS SECTIONS FOR VARIOUS SCREENED POTENTIALS

by

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B. A., Hendrix College, 1966

A MASTER'S THESIS

submitted in partial fulfillment of the

requirements for the degree

MASTER OF SCIENCE

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Manhattan, Kansas

1969

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I. INTRODUCTION

When an energetic atomic projectile travels through an amorphous target, it will normally be deflected at some angle from the original direction with some energy loss. The energy loss is due to two factors: nuclear energy loss (associated with elastic scattering from the target particles) and electronic energy loss (associated with inelastic scattering from the target particles). The elastic scattering between two atoms is dependent on the following factors: the mass of the projectile and of the target atom, the energy of the projectile, and the interaction potential between the projectile and the target atom.

The deflection angle and the differential cross section can be calculated by classical theory[1,2] and by quantum theory.[2-5] In the classical theory the orbit or path of motion and the momentum of the projectile can be specified at every point. In quantum theory, however, the momentum and position of the projectile can only be specified consistent with the uncertainty principle. The phase-shift method is exact, but it can only be used conveniently when the energy of the incoming particle is small. When the kinetic energy of the incoming particle is large compared to the scattering potential the Born approximation introduces little error. The classical approximation is valid when the following two conditions are satisfied: 1) the deBroglie wavelength of the projectile, λ, is negligible compared to the size of the scattering center, and 2) the collision is well defined within the limitations of the uncertainty principle.[5,6] According to Bohr,[7] the second condition is satisfied for the screened Bohr potential when the scattering angle, Θ, is larger than

$$\Theta^* \simeq \lambda/2\pi a$$

where a is the size of the scattering center ($a = \frac{a_0}{[Z_1^{2/3} + Z_2^{2/3}]^{1/2}}$). For an illustration of this limitation, consider a scattering of 100-kev oxygen ions ($Z_1 = 8$) with carbon atoms ($Z_2 = 6$). The above formula gives $\Theta^* = 0.25$ degrees and the classical approximation is valid for all angles greater than 0.25 degrees. On the other hand, the Born approximation is valid at small scattering angles (when the phase shifts are small). The two methods complement each other. There exists, however, a small range of scattering angles where neither procedure is valid.

Everhart[8] has calculated the scattering angle as a function of the impact parameter with the screened Bohr potential (which can be written in closed form). These calculations are based on the classical theory. There exist other forms of atomic potentials e.g. Thomas-Fermi,[9,10] Firsov,[11] and Thomas-Fermi-Dirac[12] potentials. Moliere[13,14] suggested that the Thomas-Fermi function could be approximated by a sum of three exponentials. More recently there has been increased interest in forms of atomic potentials which can be expressed in closed form.[15] Csavinszky[16] reports the modification of the Firsov potential which is expressed as the sum of two exponential terms. Roberts[17] proposes an approximation of the Thomas-Fermi function which consists of a single exponential term.[18] An empirical fitting of the Firsov potential over a large range of internuclear distance (but not valid for small r) is recently reported by Wedepohl.[19] The potentials of Csavinszky, Roberts, and Wedepohl have more desirable properties at large r. We note that the scattering calculations between atoms even with the classical model are not very extensive, and the sensitivity of the numerical results is not investigated.

It is the motivation of this work to investigate the dependence of the scattering angle and the differential cross section (with a classical

description of elastic scattering) for ions in the kev energy region on different forms of potentials. Section II contains the main points of the classical theory, and section III describes the procedure used in the present calculations. Numerical results are presented in section IV, followed by a discussion.

II. CLASSICAL THEORY OF SCATTERING

In the laboratory system the scattering is considered from a stationary target. Momentum is transferred from the projectile to the target atom, which recoils. The following quantities enter the calculations in a two-body problem: $\bar{p}_1$, $\bar{r}_1$, $\bar{p}_2$, and $\bar{r}_2$ (the momentum and position vectors of the projectile and of the target atom, respectively). However, the center of mass of the two particles is considered at rest in the center of mass system. The two-body problem can be reduced to an one-body problem provided the interaction depends only on the relative co-ordinate $\bar{r} = (\bar{r}_1 - \bar{r}_2)$. In the center of mass system the co-ordinates $\bar{r}_1$ and $\bar{r}_2$ are replaced by the co-ordinate of the center of mass $\bar{R} = (m_1\bar{r}_1 + m_2\bar{r}_2)/M$ where $M = m_1 + m_2$ and by the co-ordinate r. The motion of the center of mass, which is the motion of a free particle traveling at a constant velocity $\bar{V}_c = m_1\bar{v}/M$ where $\bar{v}$ is the initial velocity of the projectile in the laboratory system, can be separated out and one has an equivalent one-body problem with an effective mass $m = m_1m_2/M$. The experiments are done in the laboratory system and therefore we note below the relevant relations to transform the various quantities from the center of mass system to the laboratory system. The relation between the scattering angles in the laboratory system, η, and in the center of mass system, Θ, is

$$\tan \eta = \frac{\sin \Theta}{\cos \Theta + \gamma} \qquad (1)$$

γ is defined as $\left(\frac{m_1 m_3}{m_2 m_4} \cdot \frac{E}{E+Q}\right)^{1/2}$ where Q is the amount of energy converted from internal energy to kinetic energy of the emergent particle. For elastic scattering, $Q = 0$, $m_1 = m_3$, $m_2 = m_4$, γ reduces to m_1/m_2. The initial kinetic energy in the center of mass system is

$$E = m_2 E_o / M \tag{2}$$

where E_o is the initial energy of the projectile in the laboratory system. During an elastic collision the energy, T, transferred to the target atom is

$$T = T_m \sin^2(\theta/2) \tag{3}$$

where T_m is the maximum energy transfer

$$T_m = 4 m_1 m_2 E / M^2. \tag{4}$$

Finally, the connection between the differential cross sections in the laboratory system and in the center of mass system is

$$\sigma'(\gamma) = \sigma(\theta) \frac{(1+\gamma^2+2\gamma\cos\theta)^{3/2}}{|1+\gamma\cos\theta|} \tag{5}$$

The differential cross section for scattering in a given direction $\Omega(\theta,\phi)$ is defined as the number of particles scattered into a solid angle $d\Omega$ per unit time per unit incident intensity where $d\Omega$ is an element of solid angle in the direction Ω. For azimuthal symmetry in the incident beam, the differential cross section is given by

$$\frac{d\sigma}{d\Omega} = \sigma(\theta) = \frac{2\pi b\, db}{d\Omega} \tag{6}$$

where b is the impact parameter. The element of the solid angle $d\Omega$ can be written as

$$d\Omega = 2\pi \sin\theta\, d\theta \tag{7}$$

Substitution of equation (7) into equation (6) gives

$$\sigma(\theta) = \frac{b}{\sin\theta} \left| \frac{db}{d\theta} \right| \tag{8}$$

To evaluate equation (8) one must know either $b(\theta)$ or $\theta(b)$. For a central potential $V = V(r)$, the scattering angle center of mass system and the impact parameter are related by the formula

$$\Theta(b) = \pi - 2b\int_{r_o}^{\infty} \frac{dr}{r\left[\{1-(V(r)/E)\}\, r^2 - b^2\right]^{1/2}} \tag{9}$$

where r_o is the distance of closest approach. The value of r_o is defined by the largest positive root of the equation

$$\left(1 - \frac{V(r_o)}{E}\right) r_o^2 = b^2. \tag{10}$$

Except for potentials of the form $V(r) = c/r^n$, equation (9) can only be solved numerically. In addition, difficulties arise if the potential is attractive (negative) and n is greater than two. In this case r_o does not exist in equation (1)), and, in general, the deflection angle is then undefinable. Since all potentials discussed in this thesis are repulsive, this latter problem was never encountered. The integral in equation (9) can be carried out in closed form for the Coulomb potential $V(r) = Z_1 Z_2 e^2/r$, giving the familiar results:

$$\Theta = \pi - 2\cot^{-1}\left(\frac{Z_1 Z_2 e^2}{2Eb}\right) \tag{11}$$

and

$$\sigma(\Theta) = \left(\frac{Z_1 Z_2 e^2}{4E \sin^2 \frac{\Theta}{2}}\right)^2 . \tag{12}$$

Following Lindhard,[15] another potential for which the calculation of the scattering angle can be carried out in closed form is

$$V(r) = \frac{s Z_1 Z_2 e^2 a^{n-1}}{r^n}$$

where s is a scaling constant and a is a constant (dimension of length). The differential cross section is

$$d\sigma = s e^2 a^{2-2/n} (Z_1 Z_2)^{2/n} (1 - 1/n) \frac{m_1 M}{T m^{1-1/n}} \frac{\left[m_2 E/M\right]^{1-2/n}}{T^{1+1/n}}\, dT$$

T is the energy transfer and T_m is the maximum energy transfer defined in equation (4).

The Coulomb potential includes only the interaction of the two nuclei, and the screening effects of the electrons cannot adequately be described by a power potential. Other potentials have been proposed to examine the screening effect. Section III will discuss some of these potentials and describe the technique used in evaluating equation (10) and integrating equation (9). This will be followed by the presentation of the numerical results in section IV.

III. CALCULATIONAL PROCEDURE

There have been many potentials proposed which estimate the screening effects of the electrons. To investigate the effects of these potentials on the classical scattering angle and the differential cross section, one must numerically solve equation (10) for r_o and numerically evaluate the integral in equation (9). We discuss below the different forms of these potentials. The latter part of this section will deal with the procedure used in calculating the classical scattering angle and the differential cross section.

A. Screened Potentials

To approximate the screening effects of the electrons in interatomic interactions, Bohr proposed the potential

$$V(r) = \frac{Z_1 Z_2 e^2}{r} e^{-r/a} \quad . \tag{13}$$

The screening length, a, is

$$a = \frac{a_o}{[Z_1^{2/3} + Z_2^{2/3}]^{1/2}} \tag{14}$$

where a_o is the radius of the first orbit in hydrogen. The screened Bohr potential decreases too rapidly[15] for large r and is only valid in the range $r/a_o \leq 1$. Attempts[20] have been made to extend the range of validity by revising the value of the screening length, a. These revised values, however, only serve to extend the range of validity by a very small amount.

Thomas and Fermi[9] developed a statistical model to approximate the screened potential for an atom. The form of the Thomas-Fermi potential is $V(r) = \frac{Z_1 Z_2 e^2}{r} \phi(x)$. The screening factor, $\phi(x)$, is determined by the

Thomas-Fermi equation

$$d^2\phi/dx^2 = \phi^{3/2}/x^{1/2}$$
$$\phi(0) = 1 \quad , \qquad \phi(\infty) = 0 \quad , \qquad x\phi'(\infty) = 0 \tag{15}$$

The dimensionless variable, $x = \frac{Z^{1/3} r}{0.8853 a_0}$, allows the screening function to be universal for all atoms. Since equation (15) must be solved numerically, $\phi(x)$ is expressed in the form of a numerical table.[10] For the interaction between two atoms, the Thomas-Fermi potential is given by

$$V(r) = \frac{Z_1 Z_2 e^2}{r} \phi(r/a_{TF}) \tag{16}$$

where $a_{TF} = \frac{0.8853 a_0}{(Z_1^{2/3} + Z_2^{2/3})^{1/2}}$. Firsov[11] proposed a similar form of this potential,

$$V(r) = \frac{Z_1 Z_2 e^2}{r} \phi(r/a_F) \tag{17}$$

where $a_F = \frac{0.8853 a_0}{(Z_1^{1/2} + Z_2^{1/2})^{2/3}}$. There is actually very little difference in equations (16) and (17). When Z_1/Z_2 changes, the ratio a_F/a_{TF} also changes, but this variation of a_F/a_{TF} is less than ± 4 per cent, and usually considerably less.[15]

Since the Thomas-Fermi potential is not expressed in a closed form, one cannot conveniently use this potential to calculate the classical scattering angle. Moliere proposed an analytical curve fit to the Thomas-Fermi potential.[14] This approximation

$$V(r) = \frac{Z_1 Z_2 e^2}{r} \left[0.1 e^{-r/a_{TF}} + 0.55 e^{-1.2 r/a_{TF}} + 0.355 e^{-.3 r/a_{TF}} \right] \tag{18}$$

is more accurate than the screened Bohr potential set at large r and has

often been used in channeling calculations.*

Recently much work has been devoted to approximate analytical solutions of the Thomas-Fermi equation. Csavinszky[16] has proposed the trial function

$$\phi(x) = \left[a e^{-\alpha x} + b e^{-\beta x} \right]^2 \tag{19}$$

where a, b, α, and β are parameters. By the use of the variational principle, the values of these constants (a = 0.711, b = 0.2889, α = 0.175, and β = 1.6625) were found by requiring that the boundary conditions (equation (15)) be satisfied, a + b = 1, and the electron density be properly normalized. Csavinszky states that this potential varies from the Thomas-Fermi potential less than one per cent in the range $0 \leq x \leq 1.0$ and less than eight per cent in the range $1.0 \leq x \leq 2.0$. To obtain the interaction potential between two atoms, the Firsov approximation (equation (17)) was applied. Firsov limits the validity of this approximation to the range $r/a_o \leq 1.9$.

Another trial function,

$$\phi(x) = (1 + \gamma x^{1/2})\, e^{-\gamma x^{1/2}} \tag{20}$$

where γ is an undetermined constant, was suggested by Roberts.[17] The optimum value of γ = 1.7822 was determined by Anderson, Arthurs, and Robinson[18] by calculating the upper and lower bounds for total electron energy. Their criterion for a better potential was a smaller difference between the upper and lower bounds. They also checked Csavinszky's potential by the same method and concluded that Roberts' trial function was a better approximate solution to the Thomas-Fermi equation.

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*See for example C. Erginsoy, Phys. Rev. Letters 15, 360 (1965).

Recently Wedepohl[19] noted that the Thomas-Fermi screening function can be described very accurately in the range $0.3 \leq x \leq 16$ by the relation

$$\phi(x) = (317x)\, e^{-6.22x^{1/4}} \tag{21}$$

It was also noted that this form of $\phi(x)$ is not a particular solution of the Thomas-Fermi equation since $\phi(0) = 0$ and that this form is invalid for small r. When the Firsov approximation is applied, the interaction potential is given by the following relation

$$V(r) = B e^{-\alpha r^{1/4}} \tag{22}$$

where $B = 1.55(10)^{4}\ Z_1 Z_2 Z_o$ electron volts, $\alpha = 8.98 Z_o\ \text{Å}^{-1/4}$, and $Z_o = \frac{1}{4}\left(Z_1^{1/2} + Z_2^{1/2}\right)^2$. The difference between this potential and the Firsov potential is less than 1.5 per cent in the range $0.3 \geq r/a_F \geq 16$.

For three potentials (Csavinszky, Roberts, and Wedepohl), the values of the screening functions were calculated and compared in table I to the exact Thomas-Fermi screening function values.[10] We wish to investigate the behavior of the classical scattering angle and the differential cross section when each of these potentials is assumed. The numerical methods used in these calculations will be discussed in the second part of this section.

B. Numerical Procedure

We wish to examine the effects of the five screened potentials (screened Bohr, Moliere, Csavinszky, Roberts, and Wedepohl) on the classical scattering angle and the differential scattering cross section. To calculate the classical scattering angle, Θ, and the differential cross section, $\sigma(\Theta)$, for an impact parameter, b, three numerical evaluations must be performed:

TABLE I

Ratios of the screening functions of Csavinszky, ϕ_c, Roberts, ϕ_R, and Wedepohl, ϕ_w, to the Thomas-Fermi Screening function, $\phi(x)$.

x	$\phi(x)$	ϕ_c/ϕ	ϕ_R/ϕ	ϕ_w/ϕ
0.00	1.000000	1.00000	1.00000	0.00000
0.05	0.935190	1.00769	1.00391	0.74065
0.10	0.881700	1.00945	1.00934	0.86894
0.20	0.793060	1.00738	1.02119	0.95529
0.30	0.720640	1.00300	1.03315	0.98334
0.40	0.659540	0.99872	1.04481	0.99415
0.50	0.606990	0.99550	1.05601	0.99826
0.60	0.561160	0.99377	1.06670	0.99949
0.70	0.520790	0.99359	1.07685	0.99938
0.80	0.484930	0.99495	1.08646	0.99870
0.90	0.452860	0.99772	1.09554	0.99781
1.00	0.424010	1.00176	1.10411	0.99690
1.10	0.397930	1.00688	1.11218	0.99607
1.20	0.374240	1.01295	1.11979	0.99537
1.30	0.352650	1.01976	1.12692	0.99479
1.40	0.332900	1.02717	1.13360	0.99435
1.50	0.314780	1.03501	1.13984	0.99403
1.60	0.298100	1.04317	1.14567	0.99385
1.70	0.282710	1.05151	1.15109	0.99378
1.80	0.268470	1.05994	1.15614	0.99383
1.90	0.255270	1.06834	1.16082	0.99396
2.00	0.243010	1.07662	1.16511	0.99417
2.20	0.220950	1.09254	1.17271	0.99480
2.40	0.201700	1.10720	1.17901	0.99567
2.60	0.184800	1.12021	1.18410	0.99667
2.80	0.169880	1.13129	1.18804	0.99776
3.00	0.156630	1.14035	1.19099	0.99897
3.20	0.144820	1.14720	1.19293	1.00019
3.40	0.134250	1.15180	1.19392	1.00139
3.60	0.124740	1.15428	1.19414	1.00265
3.80	0.116170	1.15450	1.19368	1.00380
4.00	0.108400	1.15276	1.19222	1.00504
4.60	0.089085	1.13558	1.18417	1.00816
5.00	0.078808	1.11554	1.17595	1.00992
6.00	0.059423	1.04216	1.14749	1.01296
7.00	0.046098	0.94660	1.11056	1.01396
8.00	0.036587	0.84045	1.06799	1.01302
9.00	0.029591	0.73228	1.02184	1.01029
10.00	0.024314	0.62802	0.97372	1.00600

TABLE I (continued)

x	$\phi(x)$	ϕ_c/ϕ	ϕ_R/ϕ	ϕ_w/ϕ
15.00	0.010805	0.24558	0.73527	0.96716
25.00	0.003474	0.02307	0.38487	0.85003
50.00	0.000632	0.00002	0.07239	0.56755

1) solving equation (10) for the distance of closest approach, r_o, 2) evaluating the integral in equation (9), and 3) evaluating $db/d\theta$. The methods used to make these three evaluations will now be discussed.

1. Evaluation of r_o. The distance of closest approach, r_o, is defined by the equation

$$\left[1-\frac{V(r_o)}{E}\right]^{1/2} r_o = b \quad .$$

For a repulsive potential the left-hand side of this equation is a monotonically increasing function of r_o when $1 > V(r_o)/E$. Except for collisions which cause large deflections, the values of r_o and b vary only by a small amount. The value of r_o is found by locating the point of intersection of the curve $f(x) = (1 - (V(x)/E))^{1/2}x$ and the straight line $g(x) = b$. The operation of a mesh used to locate this point of intersection is described by the following steps. 1) First starting with $x = b$ and increasing x, if necessary, find a value of x ($x = s$) where $(1 - (V(s)/E)^{1/2}$ is real. This s is the starting value for the mesh. 2) The value of f(s) is checked and found less than (greater than) b. Then s is repeatedly increased (decreased) by the mesh size until f(s) is greater than (less than) b. At this point we know the value of r_o accurate to the value of the mesh size. 4) The mesh size is reduced and steps 2), 3), and 4) are repeated until r_o is known to the accuracy desired. If a mesh point ever coincides with the point of intersection of the two curves, the value of r_o is then known and no further calculations are needed. In the present calculations, the mesh size was varied from $0.01a_o$ to $(10^{-7})a_o$

2. Evaluation of θ. The classical scattering angle, θ, for a collision between two atoms is given by

$$\theta = \pi - 2b \int_{r_o}^{\infty} \frac{dr}{r\left(\left[1-\frac{V(r)}{E}\right] r^2 - b^2\right)^{1/2}} \quad . \qquad (9a)$$

One difficulty arises in a numerical evaluation of this equation. Since there exists a singularity at $r = r_0$ in the integrand, the numerical integration can run into trouble at this point. Recently Smith[21] suggested the use of the Gauss-Mehler quadrature to avoid this difficulty. If we substitute $x = r_0/r$ into equation (9a), it becomes

$$\Theta(b) = \pi - \frac{2b}{r_0} \int_0^1 \frac{f(x)\,dx}{(1-x^2)^{1/2}} \tag{23}$$

where

$$f(x) = \left[\frac{1-x^2}{1-[V(r_0/x)E^{-1}] - \frac{b^2x^2}{r_0^2}} \right]^{1/2} .$$

Since the singularity behaves as $(1 - x^2)^{-1/2}$ at $x = 1$, it is possible to remove this singularity by the use of a special Gaussian quadrature formula[22] derived by Mehler for integrals which have a weighting function of $(1 - u^2)^{-1/2}$. This quadrature formula is

$$\int_{-1}^{1} f(u)(1-u^2)^{-1/2}\,du = \frac{\pi}{n} \sum_{j=1}^{n} f\left(\cos \frac{2j-1}{2n}\pi\right) .$$

Since the potential is spherically symmetric, $f(x) = f(-x)$, and equation (23) can be written as

$$\Theta = \pi - \frac{b}{r_0} \int_{-1}^{1} \frac{f(x)\,dx}{(1-x^2)^{1/2}} .$$

This can be evaluated by using the Gauss-Mehler formula,

$$\Theta = \pi - \frac{b}{r_0} \frac{\pi}{n} \sum_{j=1}^{n} f\left(\cos \frac{2j-1}{2n}\pi\right)$$

If n is even,

$$\sum_{j=1}^{n} f\left(\cos \frac{2j-1}{2n}\pi\right) = 2 \sum_{j=1}^{n/2} f\left(\cos \frac{2j-1}{2n}\pi\right)$$

and the angle Θ can be approximated by the series

$$\Theta = \pi - \frac{2b}{r_0} \frac{n}{\pi} \sum_{j=1}^{n/2} f\left(\cos \frac{2j-1}{2n}\pi\right)$$

This method is very effective and is well suited for a computer. Smith calculated the deflection angles for collisions of two hydrogen atoms, assuming an interatomic potential of $V(r) = d/r^4$, and obtained an accuracy of three significant figures with only two integration points ($n = 4$). Similar accuracy is found for other repulsive potentials provided that $f(r)$ does not come close to zero for any value of $r > r_0$. This condition is satisfied for all five potentials discussed in the first part of this section. Following the suggestion of Tang and Karplus,[23] n was set equal to thirty in the present calculations.

3. Evaluation of $\sigma(\theta)$. The differential cross section, $\sigma(\theta)$, is determined by the equation

$$\sigma(\theta) = \frac{b}{\sin\theta} \frac{1}{\left| db/d\theta \right|} \tag{8a}$$

Since $\theta(b)$ cannot be expressed in a closed form, $d\theta/db$ must be numerically evaluated. This was accomplished by a four point central difference formula

$$dy_i = \frac{1}{h}\left[-\frac{1}{12} y_{i+2} + \frac{2}{3} y_{i+1} - \frac{2}{3} y_{i-1} + \frac{1}{12} y_{i+2}\right] + \mathcal{O}(h^4) \tag{24a}$$

where $h = y_{i+1} - y_i$ for all i (i.e., all points must be equidistantly spaced) and the error is approximately h^4. The derivatives at the first two points were found by a forward difference formula

$$dy_i = \frac{1}{h}\left[\frac{1}{3} y_{i+3} - \frac{3}{2} y_{i+2} + 3 y_{i+1} - \frac{11}{6} y_i\right] + \mathcal{O}(h^3) \tag{24b}$$

and the derivatives at the last two points were found by a backward difference formula

$$dy_i = \frac{1}{h}\left[-\frac{1}{3} y_{i-3} + \frac{3}{2} y_{i-2} - 3 y_{i-1} + \frac{11}{16} y_i\right] + \mathcal{O}(h^3) \tag{24c}$$

$\sigma(\theta)$ for various values of b, ranging from $0.0015a_o$ to $2.5a_o$, were calculated for each of the five potentials (screened Bohr, Moliere, Csavinszky, Roberts, and Wedepohl). The impact parameters were separated into three groups: one corresponding to small b ($0.0015a_o \leq b \leq 0.048a_o$) with $h = 0.0015a_o$ (32 points), another corresponding to central b ($0.05a_o \leq b \leq 0.6a_o$) with $h = 0.25a_o$ (19 points), and the third corresponding to large b ($0.7a_o \leq b \leq 2.5a_o$) with $h = 0.1a_o$ (21 points). At each value of b, a value of $db/d\theta$ can be found by equations (24) and the differential cross section for this value of b can then be calculated by formula (8).

In this section we examined the potentials proposed by Bohr, Moliere, Csavinszky, Roberts, and Wedepohl. In the latter part of this section the numerical methods used to calculate the distance of closest approach, the classical scattering angle, and the differential cross section were discussed. In section IV, we will show the reliability of these numerical methods by comparing present calculations to the calculations made by Everhart[3] assuming the screened Bohr potential. Results of calculations for each of the five potentials will then be presented followed by a discussion.

IV. NUMERICAL RESULTS

The classical scattering angles and the classical scattering cross sections were numerically evaluated by the methods discussed in section III for five screened potentials (Bohr, Moliere, Csavinszky, Roberts, and Wedepohl). To show the validity of the numerical methods, present calculations for the screened Bohr potential were compared to similar calculations of Everhart, Stone, and Carbone.[8] The numerical results of the scattering and cross section calculations for each potential will then be presented.

A. Comparison with Previous Calculations (Bohr potential). Everhart, Stone, and Carbone[8] presented in a tabular form their evaluations of the distance of closest approach, r_o, the impact parameter, b, and the differential cross section, $\sigma(\Theta)$, for different values of scattering angles, Θ. These calculations, made for various values of Γ/a where a is the screening length and Γ is the collision diameter, were made universal by expressing the results in dimensionless quantities: r_o/Γ, b/Γ, and $\sigma(\Theta)/\Gamma^2$. The collision diameter, $\Gamma = Z_1 Z_2 e^2/E$ where E is the energy in the center of mass system, is the distance of closest approach for a head-on collision (no screening). To compare the calculations, a value was assigned to Z_1 and Z_2 (thus fixing a). For a value of Γ/a, the values of b/Γ were used to specify E and b. These values of energy and impact parameter were used to calculate r_o and Θ, and then the values of Θ and r_o/Γ were compared to those of Everhart, Stone, and Carbone for all values of Γ/a (except $(\Gamma/a = 0)$ which corresponds to Rutherford scattering). Their results varied from the present results by an average of 0.5 per cent.

Two of these comparisons are presented in table II. This comparison was carried out for four different sets of values for Z_1 and Z_2 and it was found that the calculations varied by a maximum of 0.06 per cent. The differential cross sections $\sigma(\theta)/r^2$, were also compared, and again closs agreement (variation $\approx$ 1 per cent) was found. In addition, calculations were made to extend the tables to include small angle scattering. These are presented in tables III, IV, V, and VI. Now that the reliability of this method is established, we are ready to investigate the effects of the different potentials on the scattering angle and the cross section.

B. Results of Calculations Comparing Potentials. The scattering angle, θ, was calculated for each of the five potentials (Bohr, Moliere, Csavinszky, Roberts, and Wedepohl) for several values of energy, Z_1 and Z_2. Results of two cases (E = 21.4 kev and E = 42.9 kev) are presented in tables VII and VIII for Z_1 = 8 and Z_2 = 6. To aid comparison, for each value of b, θ_R calculated using the Roberts potential is shown along with the ratios of the angles to θ_R calculated using the other potentials.

The differential cross section was also calculated in each of the above cases. For small angles, the calculated differential cross section corresponding to the above cases are given in tables IX and X. To represent $\sigma(\theta)$ in an universal form, Lindhard, Nielsen, and Scharff[15] introduced the parameter t given by

$$t = \varepsilon^2 \sin^2 \frac{\theta}{2} \quad , \qquad \varepsilon = a'/r \tag{25}$$

where a' = 0.8853a (a is the screening length defined in equation (14)). The cross section then was written in the form

$$d\sigma = \pi a'^2 \frac{dt}{t^{3/2}} f(t)^{1/2} \tag{26}$$

TABLE II

Comparison of the present calculations of Θ and $r_o/\Gamma = \Delta$ with those of Everhart et al.[8] The ratios are given in columns 4 and 6. b and r_o are in units of $a_o = 0.53(10^{-8})$ cm and Θ is in degrees.

$\Gamma/a = 5.0$, Energy = 144.4 ev (center of mass system)

b	r_o	Θ	Θ_E/Θ	$\Delta=r_o/\Gamma$	ratio
2.0667676	2.0782	1.81060	0.9941	0.91906	0.99993
1.7841134	1.8051	3.57663	1.00653	0.79829	0.99964
1.6167821	1.6467	5.34040	1.01116	0.72823	0.99831
1.4969367	1.5353	7.10329	1.01361	0.67898	1.00002
1.3273442	1.3817	10.59636	1.01922	0.61103	0.99831
1.2007152	1.2707	14.23214	1.01179	0.56196	0.99829
1.1012208	1.1863	17.89913	1.00564	0.52464	1.00069
0.9293671	1.0476	26.44076	1.02115	0.46327	1.00374
0.7959543	0.9472	35.61025	1.01094	0.41891	1.00261
0.6037495	0.8172	54.27424	0.99495	0.36140	0.99612
0.4725978	0.7409	71.98321	1.00023	0.32764	1.00414
0.3663199	0.6884	90.11485	0.99873	0.30444	1.00185
0.1650701	0.6191	135.00760	0.99994	0.27381	0.99704
0.0002261	0.6000	179.93636	1.00035	0.26534	0.99870

$\Gamma/a = 0.2$, Energy = 3610 ev (center of mass system)

b	r_o	Θ	Θ_E/Θ	$\Delta=r_o/\Gamma$	ratio
0.8601733	0.8669	1.78958	1.00582	9.58383	1.00064
0.6322409	0.6432	3.57324	1.00749	7.11162	0.99977
0.5083253	0.5228	5.39330	1.00124	5.77959	0.99834
0.4296344	0.4468	7.16238	1.00525	4.93981	1.00004
0.3283311	0.3499	10.71804	1.00483	3.86800	1.00052
0.2641121	0.2891	14.43917	0.99729	3.19577	0.99819
0.2206964	0.2484	18.10185	0.99437	2.74574	0.99791
0.1564773	0.1891	26.97016	1.00111	2.09020	0.99990
0.1193971	0.1557	35.95865	1.00115	1.72113	1.00515
0.0782387	0.1202	54.03629	0.99933	1.32937	1.00799
0.0556263	0.1024	71.97532	1.00034	1.13167	0.99852

TABLE II (continued)

$\Gamma/a = 0.2$, Energy = 3610 ev (center mass system)

b	r_o	θ	θ_E/θ	$\Delta=r_o/\Gamma$	ratio
0.04707022	0.0919	89.93896	1.00068	1.01558	1.00435
0.01691140	0.0795	135.09512	0.99930	0.87864	0.99927
0.0000090	0.0764	179.97470	1.00014	0.84458	1.00050

TABLE III

$\sigma(\theta)/\Gamma^2$ for different values of impact parameter, b, for the screened Bohr potential. $\Gamma = Z_1 Z_2 e^2/E$. θ is in degrees. The number in parentheses after an entry is the power of 10 to be multiplied by it.

$\Gamma/a = 0.1$

b/Γ	r_o/Γ	θ	$\sigma(\theta)/\Gamma^2$
67.5552	67.5558	0.0034	0.1421(12)
64.8530	64.8537	0.0046	0.1251(12)
62.1508	62.1518	0.0060	0.5239(11)
59.4485	59.4499	0.0082	0.2684(11)
56.7463	56.7481	0.0109	0.1440(11)
54.0441	54.0464	0.0147	0.7385(10)
51.3419	51.3449	0.0198	0.3853(10)
48.6397	48.6436	0.0268	0.1975(10)
45.9375	45.9426	0.0364	0.1012(10)
43.2353	43.2419	0.0493	0.5138(9)
40.5331	40.5418	0.0672	0.2588(9)
37.8309	37.8423	0.0915	0.1280(9)
35.1287	35.1436	0.1255	0.6296(8)
32.4265	32.4460	0.1719	0.3069(8)
29.7243	29.7498	0.2369	0.1449(8)
27.0221	27.0555	0.3287	0.6756(7)
24.3199	24.3637	0.4579	0.3063(7)
21.6177	21.6750	0.6443	0.1336(7)
18.9155	18.9905	0.9161	0.5596(6)
16.2133	16.3114	1.3210	0.2235(6)
13.5111	13.6395	1.9440	0.8109(5)

$\Gamma/a = 0.2$

b/Γ	r_o/Γ	θ	$\sigma(\theta)/\Gamma^2$
36.4798	36.4801	0.0037	0.3703(11)
35.1287	35.1291	0.0050	0.2261(11)
33.7776	33.7782	0.0067	0.1110(11)
32.4265	32.4272	0.0091	0.5929(10)
31.0754	31.0764	0.0121	0.3110(10)
29.7243	29.7256	0.0165	0.1662(10)
28.3732	28.3749	0.0219	0.8883(9)

TABLE III (continued)

		/a = 0.2	
b/λ	r_o/λ	θ	$\sigma(\theta)/\lambda^2$
27.0221	27.0243	0.0296	0.4541(9)
25.6709	25.6739	0.0400	0.2401(9)
24.3199	24.3237	0.0538	0.1245(9)
22.9688	22.9738	0.0728	0.6330(8)
21.6177	21.6243	0.0987	0.3211(8)
20.2666	20.2752	0.1343	0.1616(8)
18.9155	18.9268	0.1830	0.8055(7)
17.5643	17.5792	0.2502	0.3968(7)
16.2132	16.2327	0.3430	0.1926(7)
14.8621	14.8876	0.4724	0.9159(6)
13.5110	13.5444	0.6541	0.4270(6)
12.1599	12.2036	0.9113	0.1941(6)
10.8088	10.8659	1.2793	0.8608(5)
9.4577	9.5323	1.8141	0.3632(5)

TABLE IV

$\sigma(\theta)/\Gamma^2$ for different values of impact parameter, b, for the screened Bohr potential. $\Gamma = Z_1 Z_2 e^2/E$. θ is in degrees. The number in parentheses after an entry is the power of 10 to be multiplied by it.

$\Gamma/a = 0.5$

b/Γ	r_o/Γ	θ	$\sigma(\theta)/\Gamma^2$
15.6728	15.6730	0.0053	0.3930(10)
15.1324	15.1326	0.0070	0.1790(10)
14.5919	14.5923	0.0095	0.9592(9)
14.0515	14.0519	0.0127	0.5247(9)
13.5110	13.5116	0.0170	0.2840(9)
12.9706	12.9714	0.0228	0.1537(9)
12.4302	12.4312	0.0304	0.8212(8)
11.8897	11.8910	0.0408	0.4286(8)
11.3493	11.3510	0.0549	0.2259(8)
10.8088	10.8111	0.0738	0.1182(8)
10.2684	10.2713	0.0996	0.6131(7)
9.7280	9.7318	0.1344	0.3180(7)
9.1875	9.1926	0.1817	0.1629(7)
8.6471	8.6537	0.2464	0.8290(6)
8.1066	8.1153	0.3345	0.4190(6)
7.5662	7.5775	0.4553	0.2094(6)
7.0257	7.0406	0.6213	0.1034(6)
6.4853	6.5047	0.8508	0.5035(5)
5.9449	5.9702	1.1689	0.2415(5)
5.4044	5.4375	1.6134	0.1143(5)
4.8640	4.9072	2.2391	0.5247(4)

$/a = 1.0$

b/Γ	r_o/Γ	θ	$\sigma(\theta)/\Gamma^2$
8.3768	8.3770	0.0059	0.7281(9)
8.1066	8.1068	0.0079	0.4099(9)
7.8364	7.8366	0.0105	0.2141(9)
7.5662	7.5664	0.0141	0.1151(9)
7.2960	7.2963	0.0189	0.6271(8)
7.0257	7.0262	0.0252	0.3346(8)

TABLE IV (continued)

$\Gamma/a = 1.0$

b/Γ	r_o/Γ	θ	$\sigma(\theta)/\Gamma^2$
6.7555	6.7561	0.0339	0.1774(8)
6.4853	6.4861	0.0454	0.9545(7)
6.2151	6.2161	0.0608	0.5105(7)
5.9449	5.9462	0.0816	0.2680(7)
5.6746	5.6763	0.1098	0.1410(7)
5.4044	5.4067	0.1476	0.7422(6)
5.1342	5.1371	0.1987	0.3867(6)
4.8640	4.8678	0.2681	0.1995(6)
4.5938	4.5988	0.3626	0.1026(6)
4.3235	4.3301	0.4907	0.5258(5)
4.0533	4.0619	0.6650	0.2664(5)
3.7831	3.7944	0.9036	0.1336(5)
3.5129	3.5276	1.2305	0.6645(4)
3.2427	3.2619	1.6797	0.3284(4)
2.9724	2.9975	2.2997	0.1589(4)

TABLE V

$\sigma(\theta)/\Gamma^2$ for different values of impact parameter, b, for the screened Bohr potential. $\Gamma = z_1 z_2 e^2/E$. θ is in degrees. The number in parentheses after an entry is the power of 10 to be multiplied by it.

$\Gamma/a = 2.0$

b/Γ	r_o/Γ	θ	$\sigma(\theta)/\Gamma^2$
4.4586	4.4587	0.0068	0.1836(9)
4.3235	4.3236	0.0089	0.7898(8)
4.1884	4.1885	0.0119	0.4499(8)
4.0533	4.0535	0.0159	0.2482(8)
3.9182	3.9184	0.0212	0.1347(8)
3.7831	3.7833	0.0282	0.7256(7)
3.6480	3.6483	0.0378	0.3870(7)
3.5129	3.5133	0.0506	0.2096(7)
3.3778	3.3783	0.0676	0.1123(7)
3.2426	3.2434	0.0907	0.5972(6)
3.1075	3.1085	0.1215	0.3192(6)
2.9724	2.9737	0.1629	0.1690(6)
2.8373	2.8390	0.2188	0.8880(5)
2.7022	2.7044	0.2944	0.4665(5)
2.5671	2.5700	0.3961	0.2440(5)
2.4320	2.4358	0.5337	0.1268(5)
2.2969	2.3019	0.7199	0.6558(4)
2.1618	2.1683	0.9723	0.3367(4)
2.0267	2.0352	1.3151	0.1719(4)
1.8915	1.9027	1.7804	0.8769(3)
1.7564	1.7710	2.4138	0.4408(3)

$\Gamma/a = 5.0$

b/Γ	r_o/Γ	θ	$\sigma(\theta)/\Gamma^2$
1.9456	1.9456	0.0071	0.2386(8)
1.8915	1.8916	0.0095	0.1244(8)
1.8375	1.8376	0.0126	0.7290(7)
1.7835	1.7835	0.0167	0.3947(7)
1.7294	1.7295	0.0224	0.2109(7)
1.6754	1.6755	0.0298	0.1171(7)
1.6213	1.6215	0.0396	0.6409(6)

TABLE V (continued)

$\Gamma/a = 5.0$

b/Γ	r_o/Γ	θ	$\sigma(\theta)/\Gamma^2$
1.5673	1.5675	0.0529	0.3437(6)
1.5132	1.5135	0.0707	0.1854(6)
1.4592	1.4595	0.0944	0.1001(6)
1.4051	1.4056	0.1262	0.5385(5)
1.3511	1.3517	0.1688	0.2898(5)
1.2971	1.2978	0.2257	0.1548(5)
1.2430	1.2440	0.3025	0.8243(4)
1.1890	1.1903	0.4052	0.4386(4)
1.1349	1.1366	0.5434	0.2323(4)
1.0809	1.0831	0.7290	0.1227(4)
1.0268	1.0297	0.9786	0.6462(3)
0.9728	0.9766	1.3138	0.3393(3)
0.9188	0.9237	1.7644	0.1783(3)
0.8647	0.8711	2.3689	0.9332(2)

TABLE VI

$\sigma(\theta)/\Gamma^2$ for different values of impact parameter, b, for the screened Bohr potential. $\Gamma = z_1 z_2 e^2/E$. θ is in degrees. The number in parentheses after an entry is the power of 10 to be multiplied by it.

$\Gamma/a = 10.0$

b/Γ	r_o/Γ	θ	$\sigma(\theta)/\Gamma^2$
1.0268	1.0269	0.0081	0.4989(7)
0.9998	0.9998	0.0107	0.2700(7)
0.9728	0.9728	0.0142	0.1490(7)
0.9458	0.9458	0.0190	0.8152(6)
0.9188	0.9188	0.0252	0.4529(6)
0.8917	0.8918	0.0335	0.2466(6)
0.8647	0.8648	0.0447	0.1340(6)
0.8377	0.8378	0.0594	0.7340(5)
0.8107	0.8108	0.0793	0.3963(5)
0.7836	0.7838	0.1058	0.2155(5)
0.7566	0.7569	0.1411	0.1172(5)
0.7296	0.7299	0.1883	0.6315(4)
0.7026	0.7030	0.2515	0.3401(4)
0.6756	0.6761	0.3361	0.1828(4)
0.6485	0.6493	0.4494	0.9807(3)
0.6215	0.6225	0.6009	0.5258(3)
0.5945	0.5958	0.8035	0.2811(3)
0.5675	0.5692	1.0746	0.1501(3)
0.5404	0.5426	1.4364	0.8009(2)
0.5134	0.5163	1.9196	0.4283(2)
0.4864	0.4901	2.5628	0.2288(2)

TABLE VII

For $Z_1 = 8$, $Z_2 = 6$, and E = 42,800 ev (E_{Lab} = 100 kev) calculated scattering angle with Roberts potential, Θ_R. The impact parameter, b, is in units of $a_o = 0.53(10\text{-}8)$ cm. Columns 3-6 represent the ratios of the scattering angles calculated with the Bohr potential (B), the Csavinszky potential (C), the Moliere potential (M), and the Wedepohl potential (W) to the corresponding value of Θ_R. Θ is in degrees. The number in parentheses after an entry is the power of 10 to be multiplied by it.

b	Θ_R	Θ_B/Θ_R	Θ_C/Θ_R	Θ_M/Θ_R	Θ_W/Θ_R
2.5000	0.4971(-1)	0.0568	0.8576	1.0849	0.9046
2.4000	0.5616(-1)	0.0671	0.8780	1.0821	0.8940
2.3000	0.6333(-1)	0.0794	0.9004	1.0817	0.8891
2.2000	0.7200(-1)	0.0922	0.9160	1.0711	0.8780
2.1000	0.8183(-1)	0.1103	0.9334	1.0664	0.8702
2.0000	0.9357(-1)	0.1296	0.9490	1.0561	0.8601
1.9000	0.1071	0.1544	0.9637	1.0504	0.8564
1.8000	0.1235	0.1800	0.9753	1.0378	0.8502
1.7000	0.1430	0.2091	0.9841	1.0256	0.8437
1.6000	0.1665	0.2447	0.9895	1.0119	0.8374
1.5000	0.1947	0.2834	0.9943	0.9982	0.8340
1.4000	0.2292	0.3295	0.9948	0.9860	0.8322
1.3000	0.2718	0.3798	0.9936	0.9742	0.8301
1.2000	0.3252	0.4352	0.9876	0.9624	0.8300
1.1000	0.3923	0.4973	0.9792	0.9524	0.8314
1.0000	0.4791	0.5646	0.9672	0.9446	0.8339
0.9000	0.5925	0.6369	0.9526	0.9405	0.8385
0.8000	0.7445	0.7130	0.9365	0.9396	0.8447
0.7000	0.9539	0.7917	0.9198	0.9426	0.8541
0.6000	0.1252(1)	0.8703	0.9063	0.9510	0.8676
0.5000	0.1699(1)	0.9448	0.8955	0.9613	0.8837
0.4750	0.1844(1)	0.9623	0.8951	0.9650	0.8887
0.4500	0.2010(1)	0.9794	0.8939	0.9678	0.8934
0.4250	0.2197(1)	0.9957	0.8947	0.9714	0.8989
0.4000	0.2411(1)	1.0108	0.8957	0.9749	0.9050
0.3750	0.2657(1)	1.0249	0.8969	0.9781	0.9107
0.3500	0.2942(1)	1.0381	0.9000	0.9815	0.9169
0.3250	0.3276(1)	1.0501	0.9037	0.9843	0.9236
0.3000	0.3671(1)	1.0603	0.9087	0.9869	0.9302
0.2750	0.4142(1)	1.0697	0.9147	0.9897	0.9378
0.2500	0.4717(1)	1.0767	0.9219	0.9916	0.9446
0.2250	0.5426(1)	1.0819	0.9303	0.9933	0.9513
0.2000	0.6320(1)	1.0853	0.9397	0.9948	0.9580
0.1750	0.7479(1)	1.0860	0.9503	0.9961	0.9639

TABLE VII (continued)

b	θ_R	θ_B/θ_R	θ_C/θ_R	θ_M/θ_R	θ_W/θ_R
0.1500	0.9033(1)	1.0847	0.9618	0.9975	0.9687
0.1250	0.1122(2)	1.0800	0.9729	0.9985	0.9704
0.1000	0.1450(2)	1.0728	0.9845	1.0002	0.9679
0.0750	0.1991(2)	1.0624	0.9945	1.0018	0.9573
0.0500	0.3045(2)	1.0485	1.0016	1.0035	0.9317
0.0480	0.3173(2)	1.0472	1.0022	1.0036	0.9288
0.0465	0.3275(2)	1.0464	1.0025	1.0040	0.9266
0.0450	0.3385(2)	1.0453	1.0026	1.0038	0.9241
0.0435	0.3500(2)	1.0443	1.0029	1.0039	0.9217
0.0420	0.3624(2)	1.0432	1.0033	1.0041	0.9190
0.0405	0.3755(2)	1.0423	1.0034	1.0041	0.9164
0.0390	0.3895(2)	1.0414	1.0038	1.0042	0.9137
0.0375	0.4044(2)	1.0403	1.0039	1.0044	0.9110
0.0360	0.4206(2)	1.0392	1.0040	1.0041	0.9079
0.0345	0.4378(2)	1.0380	1.0042	1.0044	0.9051
0.0330	0.4565(2)	1.0368	1.0042	1.0042	0.9018
0.0315	0.4765(2)	1.0358	1.0045	1.0043	0.8989
0.0300	0.4982(2)	1.0346	1.0044	1.0043	0.8958
0.0285	0.5217(2)	1.0335	1.0045	1.0044	0.8929
0.0270	0.5473(2)	1.0322	1.0046	1.0044	0.8897
0.0255	0.5752(2)	1.0309	1.0046	1.0043	0.8867
0.0240	0.6057(2)	1.0297	1.0046	1.0043	0.8841
0.0225	0.6392(2)	1.0282	1.0045	1.0041	0.8815
0.0210	0.6760(2)	1.0268	1.0043	1.0041	0.8791
0.0195	0.7165(2)	1.0254	1.0041	1.0039	0.8773
0.0180	0.7612(2)	1.0238	1.0041	1.0038	0.8760
0.0165	0.8108(2)	1.0223	1.0038	1.0036	0.8755
0.0150	0.8656(2)	1.0207	1.0036	1.0035	0.8762
0.0135	0.9266(2)	1.0188	1.0033	1.0032	0.8780
0.0120	0.9943(2)	1.0170	1.0031	1.0030	0.8817
0.0105	0.1069(3)	1.0150	1.0028	1.0027	0.8875
0.0090	0.1152(3)	1.0130	1.0024	1.0024	0.8957
0.0075	0.1243(3)	1.0107	1.0020	1.0020	0.9069
0.0060	0.1342(3)	1.0085	1.0016	1.0016	0.9213
0.0045	0.1448(3)	1.0063	1.0012	1.0012	0.9388
0.0030	0.1562(3)	1.0040	1.0008	1.0008	0.9587
0.0015	0.1680(3)	1.0019	1.0004	1.0004	0.9797

TABLE VIII

For $Z_1 = 8$, $Z_2 = 6$, and E = 21,440 ev (E_{Lab} = 50 kev) calculated scattering with Roberts potential, Θ_R. The impact parameter, b, is in units of $a_o = 0.53(10^{-8})$ cm. Columns 3-6 represent the ratios of the scattering angles calculated with the Bohr potential (B), the Csavinszky potential (C), the Moliere potential (M), and the Wedepohl potential (W) to the corresponding value of Θ_R. The number in parentheses after an entry is the power of 10 to be multiplied by it.

b	Θ_R	Θ_B/Θ_R	Θ_C/Θ_R	Θ_M/Θ_R	Θ_W/Θ_R
2.5000	0.9937(-1)	0.0558	0.8584	1.0862	0.9049
2.4000	0.1122	0.0663	0.8768	1.0815	0.8938
2.3000	0.1267	0.0785	0.8977	1.0793	0.8867
2.2000	0.1438	0.0933	0.9170	1.0725	0.8767
2.1000	0.1635	0.1113	0.9345	1.0660	0.8699
2.0000	0.1869	0.1308	0.9489	1.0571	0.8618
1.9000	0.2143	0.1529	0.9626	1.0484	0.8546
1.8000	0.2468	0.1803	0.9745	1.0368	0.8485
1.7000	0.2856	0.2100	0.9837	1.0253	0.8430
1.6000	0.3321	0.2446	0.9903	1.0129	0.8383
1.5000	0.3885	0.2845	0.9943	0.9991	0.8350
1.4000	0.4571	0.3292	0.9955	0.9871	0.8330
1.3000	0.5423	0.3800	0.9930	0.9737	0.8310
1.2000	0.6484	0.4360	0.9874	0.9622	0.8305
1.1000	0.7823	0.4977	0.9789	0.9527	0.8313
1.0000	0.9544	0.5647	0.9674	0.9450	0.8345
0.9000	0.1179(1)	0.6372	0.9535	0.9405	0.8387
0.8000	0.1481(1)	0.7131	0.9374	0.9397	0.8453
0.7000	0.1894(1)	0.7911	0.9215	0.9430	0.8547
0.6000	0.2482(1)	0.8690	0.9069	0.9506	0.8677
0.5000	0.3361(1)	0.9421	0.8970	0.9612	0.8838
0.4750	0.3648(1)	0.9595	0.8961	0.9644	0.8885
0.4500	0.3971(1)	0.9759	0.8954	0.9677	0.8936
0.4250	0.4339(1)	0.9916	0.8956	0.9710	0.8989
0.4000	0.4757(1)	1.0067	0.8964	0.9742	0.9045
0.3750	0.5238(1)	1.0207	0.8980	0.9775	0.9103
0.3500	0.5794(1)	1.0337	0.9007	0.9805	0.9165
0.3250	0.6445(1)	1.0451	0.9042	0.9834	0.9229
0.3000	0.7211(1)	1.0554	0.9089	0.9864	0.9296
0.2750	0.8127(1)	1.0642	0.9146	0.9886	0.9363
0.2500	0.9235(1)	1.0712	0.9213	0.9909	0.9432
0.2250	0.1060(2)	1.0766	0.9292	0.9928	0.9501
0.2000	0.1232(2)	1.0802	0.9383	0.9944	0.9568
0.1750	0.1453(2)	1.0812	0.9479	0.9958	0.9626

TABLE VIII (continued)

b	θ_R	θ_B/θ_R	θ_C/θ_R	θ_M/θ_R	θ_W/θ_R
0.1500	0.1748(2)	1.0802	0.9583	0.9969	0.9677
0.1250	0.2159(2)	1.0764	0.9689	0.9979	0.9706
0.1000	0.2764(2)	1.0702	0.9794	0.9991	0.9709
0.0750	0.3738(2)	1.0607	0.9888	1.0004	0.9665
0.0500	0.5510(2)	1.0476	0.9960	1.0016	0.9571
0.0480	0.5714(2)	1.0463	0.9965	1.0017	0.9562
0.0465	0.5876(2)	1.0452	0.9968	1.0017	0.9556
0.0450	0.6045(2)	1.0443	0.9971	1.0018	0.9549
0.0435	0.6223(2)	1.0432	0.9973	1.0018	0.9542
0.0420	0.6410(2)	1.0422	0.9976	1.0019	0.9537
0.0405	0.6606(2)	1.0412	0.9980	1.0020	0.9532
0.0390	0.6813(2)	1.0400	0.9982	1.0020	0.9527
0.0375	0.7030(2)	1.0389	0.9984	1.0020	0.9522
0.0360	0.7259(2)	1.0377	0.9987	1.0020	0.9518
0.0345	0.7500(2)	1.0365	0.9989	1.0020	0.9515
0.0330	0.7755(2)	1.0353	0.9991	1.0020	0.9512
0.0315	0.8023(2)	1.0340	0.9992	1.0020	0.9511
0.0300	0.8307(2)	1.0327	0.9994	1.0020	0.9512
0.0285	0.8606(2)	1.0314	0.9996	1.0020	0.9513
0.0270	0.8922(2)	1.0299	0.9997	1.0020	0.9516
0.0255	0.9256(2)	1.0285	0.9998	1.0019	0.9521
0.0240	0.9608(2)	1.0270	1.0000	1.0019	0.9529
0.0225	0.9980(2)	1.0255	1.0001	1.0019	0.9538
0.0210	0.1037(3)	1.0239	1.0001	1.0018	0.9550
0.0195	0.1079(3)	1.0222	1.0002	1.0017	0.9565
0.0180	0.1122(3)	1.0206	1.0002	1.0016	0.9583
0.0165	0.1168(3)	1.0189	1.0002	1.0015	0.9604
0.0150	0.1216(3)	1.0171	1.0003	1.0014	0.9629
0.0135	0.1266(3)	1.0154	1.0003	1.0013	0.9657
0.0120	0.1319(3)	1.0136	1.0003	1.0012	0.9688
0.0105	0.1373(3)	1.0118	1.0002	1.0010	0.9722
0.0090	0.1430(3)	1.0100	1.0002	1.0009	0.9758
0.0075	0.1488(3)	1.0082	1.0002	1.0007	0.9797
0.0060	0.1549(3)	1.0064	1.0002	1.0006	0.9838
0.0045	0.1610(3)	1.0047	1.0001	1.0004	0.9879
0.0030	0.1673(3)	1.0031	1.0001	1.0003	0.9921
0.0015	0.1736(3)	1.0015	1.0000	1.0001	0.9961

TABLE IX

Calculated differential cross sections for the Bohr potential (B), the Csavinszky potential (C), the Roberts potential (R), the Moliere potential (M), and the Wedepohl potential (W) in units of a_o^2 ($a_o = 0.53(10^{-8})$cm). The values of impact parameter, b, are in units of a_o. E = 42.9 kev (E_{Lab} = 100 kev), $Z_1 = 8$, and $Z_2 = 6$. The number in parentheses after an entry is the power of 10 to be multiplied by it.

b	$\sigma_B(\theta)$	$\sigma_C(\theta)$	$\sigma_R(\theta)$	$\sigma_M(\theta)$	$\sigma_W(\theta)$
2.500	0.3615(9)	0.3088(7)	0.2592(7)	0.2372(7)	0.3788(7)
2.400	0.1711(9)	0.2227(7)	0.2233(7)	0.1734(7)	0.2725(7)
2.300	0.1076(9)	0.1598(7)	0.1598(7)	0.1357(7)	0.2068(7)
2.200	0.5532(8)	0.1139(7)	0.1088(7)	0.1003(7)	0.1541(7)
2.100	0.2833(8)	0.7932(6)	0.7853(6)	0.7319(6)	0.1132(7)
2.000	0.1459(8)	0.5532(6)	0.5581(6)	0.5279(6)	0.7990(6)
1.900	0.7547(7)	0.3846(6)	0.3927(6)	0.3800(6)	0.5572(6)
1.800	0.4075(7)	0.2628(6)	0.2682(6)	0.2719(6)	0.3290(6)
1.700	0.2046(7)	0.1802(6)	0.1826(6)	0.1897(6)	0.2710(6)
1.600	0.1038(7)	0.1213(6)	0.1229(6)	0.1318(6)	0.1822(6)
1.500	0.5225(6)	0.8099(5)	0.8137(5)	0.8889(5)	0.1190(6)
1.400	0.2577(6)	0.5317(5)	0.5259(5)	0.5832(5)	0.7710(5)
1.300	0.1279(6)	0.3417(5)	0.3303(5)	0.3744(5)	0.4834(5)
1.200	0.6184(5)	0.2172(5)	0.2034(5)	0.2343(5)	0.2939(5)
1.100	0.2932(5)	0.1338(5)	0.1213(5)	0.1408(5)	0.1735(5)
1.000	0.1362(5)	0.7973(4)	0.6955(4)	0.8044(4)	0.9801(4)
0.900	0.6170(4)	0.4558(4)	0.3831(4)	0.4385(4)	0.5299(4)
0.800	0.2695(4)	0.2467(4)	0.1998(4)	0.2256(4)	0.2699(4)
0.700	0.1127(4)	0.1237(4)	0.9795(3)	0.1076(4)	0.1276(4)
0.600	0.4497(3)	0.5686(3)	0.4466(3)	0.4747(3)	0.5587(3)
0.500	0.1624(3)	0.2299(3)	0.1784(3)	0.1868(3)	0.2160(3)
0.475	0.1201(3)	0.1750(3)	0.1352(3)	0.1419(3)	0.1621(3)
0.450	0.9130(2)	0.1314(3)	0.1048(3)	0.1078(3)	0.1233(3)
0.425	0.6843(2)	0.9824(2)	0.7959(2)	0.8098(2)	0.9181(2)
0.400	0.5048(2)	0.7324(2)	0.5939(2)	0.6033(2)	0.6785(2)
0.375	0.3678(2)	0.5318(2)	0.4382(2)	0.4429(2)	0.4962(2)
0.350	0.2641(2)	0.3785(2)	0.3179(2)	0.3203(2)	0.3541(2)
0.325	0.1863(2)	0.2640(2)	0.2250(2)	0.2267(2)	0.2479(2)
0.300	0.1286(2)	0.1797(2)	0.1561(2)	0.1565(2)	0.1692(2)
0.275	0.8668(1)	0.1190(2)	0.1053(2)	0.1055(2)	0.1127(2)
0.250	0.5680(1)	0.7593(1)	0.6859(1)	0.6883(1)	0.7300(1)
0.225	0.3585(1)	0.4674(1)	0.4311(1)	0.4321(1)	0.4542(1)
0.200	0.2165(1)	0.2737(1)	0.2579(1)	0.2584(1)	0.2697(1)
0.175	0.1233(1)	0.1508(1)	0.1452(1)	0.1452(1)	0.1513(1)
0.150	0.6508	0.7711	0.7547	0.7544	0.7898
0.125	0.3101	0.3548	0.3531	0.3521	0.3742
0.100	0.1278	0.1415	0.1427	0.1418	0.1549

TABLE IX (continued)

b	$6_B(\theta)$	$6_c(\theta)$	$6_R(\theta)$	$6_M(\theta)$	$6_W(\theta)$
0.075	0.4227(-1)	0.4549(-1)	0.4612(-1)	0.4578(-1)	0.5246(-1)
0.050	0.9436(-2)	0.9887(-2)	0.1003(-1)	0.9927(-2)	0.1232(-1)

TABLE X

Calculated differential cross sections for the Bohr potential (B), the Csavinszky potential (C), the Roberts potential (R), the Moliere potential (M), and the Wedepohl potential (W) in units of a_o^2 ($a_o = 0.53(10^{-8})$ cm). The values of impact parameter, b, are in units of a_o. E = 21.4 kev (E_{Lab} = 50 kev), Z_1 = 8, and Z_2 = 6. The number in parentheses after an entry is the power of 10 to be multiplied by it.

b	$\sigma_B(\theta)$	$\sigma_C(\theta)$	$\sigma_R(\theta)$	$\sigma_M(\theta)$	$\sigma_W(\theta)$
2.500	0.8773(8)	0.7970(6)	0.6713(6)	0.6111(6)	0.9597(6)
2.400	0.4909(8)	0.5716(6)	0.5317(6)	0.4467(6)	0.6842(6)
2.300	0.2585(8)	0.3970(6)	0.3785(6)	0.3364(6)	0.5232(6)
2.200	0.1317(8)	0.2812(6)	0.2740(6)	0.2504(6)	0.3851(6)
2.100	0.6952(7)	0.1996(6)	0.1968(6)	0.1834(6)	0.2782(6)
2.000	0.3778(7)	0.1394(6)	0.1392(6)	0.1326(6)	0.2009(6)
1.900	0.1926(7)	0.9623(5)	0.9786(5)	0.9578(5)	0.1418(6)
1.800	0.9903(6)	0.6613(5)	0.6757(5)	0.6816(5)	0.9851(5)
1.700	0.5166(6)	0.4523(5)	0.4614(5)	0.4759(5)	0.6776(5)
1.600	0.2598(6)	0.3049(5)	0.3094(5)	0.3300(5)	0.4544(5)
1.500	0.1310(6)	0.2034(5)	0.2045(5)	0.2227(5)	0.2989(5)
1.400	0.6511(5)	0.1338(5)	0.1320(5)	0.1470(5)	0.1932(5)
1.300	0.3192(5)	0.8635(4)	0.8312(4)	0.9473(4)	0.1214(5)
1.200	0.1551(5)	0.5468(4)	0.5124(4)	0.5884(4)	0.7429(4)
1.100	0.7394(4)	0.3369(4)	0.3058(4)	0.3537(4)	0.4370(4)
1.000	0.3442(4)	0.2011(4)	0.1761(4)	0.2038(4)	0.2477(4)
0.900	0.1559(4)	0.1152(4)	0.9704(3)	0.1112(4)	0.1341(4)
0.800	0.6846(3)	0.6238(3)	0.5077(3)	0.5720(3)	0.6837(3)
0.700	0.2877(3)	0.3149(3)	0.2496(3)	0.2744(3)	0.3252(3)
0.600	0.1152(3)	0.1463(3)	0.1140(3)	0.1219(3)	0.1430(3)
0.500	0.4222(2)	0.5867(2)	0.4601(2)	0.4803(2)	0.5556(2)
0.475	0.3152(2)	0.4441(2)	0.3508(2)	0.3628(2)	0.4166(2)
0.450	0.2386(2)	0.3384(2)	0.2703(2)	0.2777(2)	0.3171(2)
0.425	0.1783(2)	0.2546(2)	0.2056(2)	0.2102(2)	0.2384(2)
0.400	0.1320(2)	0.1893(2)	0.1543(2)	0.1569(2)	0.1767(2)
0.375	0.9653(1)	0.1381(2)	0.1141(2)	0.1156(2)	0.1290(2)
0.350	0.6955(1)	0.9876(1)	0.8279(1)	0.8371(1)	0.9242(1)
0.325	0.4927(1)	0.6920(1)	0.5895(1)	0.5930(1)	0.6493(1)
0.300	0.3416(1)	0.4730(1)	0.4102(1)	0.4122(1)	0.4468(1)
0.275	0.2315(1)	0.3146(1)	0.2778(1)	0.2790(1)	0.2991(1)
0.250	0.1523(1)	0.2025(1)	0.1824(1)	0.1828(1)	0.1940(1)
0.225	0.9667	0.1254(1)	0.1153(1)	0.1155(1)	0.1215(1)
0.200	0.5885	0.7419	0.6950	0.6962	0.7284
0.175	0.3387	0.4443	0.3954	0.3959	0.4126
0.150	0.1813	0.2449	0.2087	0.2089	0.2179
0.125	0.8829(-1)	0.1013	0.9988(-1)	0.9979(-1)	0.1049

TABLE X (continued)

b	$\sigma_B(\theta)$	$\sigma_C(\theta)$	$\sigma_R(\theta)$	$\sigma_M(\theta)$	$\sigma_W(\theta)$
0.100	0.3768(-1)	0.4187(-1)	0.4178(-1)	0.4165(-1)	0.4449(-1)
0.075	0.1348(-1)	0.1450(-1)	0.1457(-1)	0.1451(-1)	0.1585(-1)
0.050	0.3601(-2)	0.3743(-2)	0.3769(-2)	0.3750(-2)	0.4168(-2)

where $f(t^{1/2})$ is a scaling factor called the reduced cross section. The factor $t^{-3/2}$ was introduced so that for a potential proportional to r^{-2}, $f(t^{1/2})$ is constant. In the present calculations,

$$\sigma(\theta) = \frac{d\sigma}{d\Omega} = \frac{d\sigma}{2\pi \sin\theta d\theta} \tag{27}$$

is evaluated by equations (24). From equation (25)

$$dt = \varepsilon^2 2 \sin\frac{\theta}{2}\cos\frac{\theta}{2}\cdot\frac{1}{2} = \frac{1}{2}\varepsilon^2 \sin\theta$$

Substituting the above equation into equation (27) we get

$$\frac{d\sigma}{dt} = \frac{4\pi\sigma(\theta)}{\varepsilon^2}$$

and $f(t^{1/2})$ is given by the relation

$$f(t^{1/2}) = \frac{8t^{3/2}\sigma(\theta)}{a'^2\varepsilon^2} \tag{28}$$

Except for potentials of the form, $V(r) = c/r^n$, $f(t^{1/2})$ must be evaluated numerically. The calculated values of θ and $\sigma(\theta)$ were substituted into equations (25) and (27) to evaluate $f(t^{1/2})$. Results of these calculations are presented in figures 1 and 2 and in tables XI through XV. These curves can be used for any combination of Z_1, Z_2 and E.*

This completes a detailed comparison of scattering angle and differential cross section for various forms of the interatomic potentials. The discussion and conclusion are in the next section.

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*Where the classical calculations are valid.

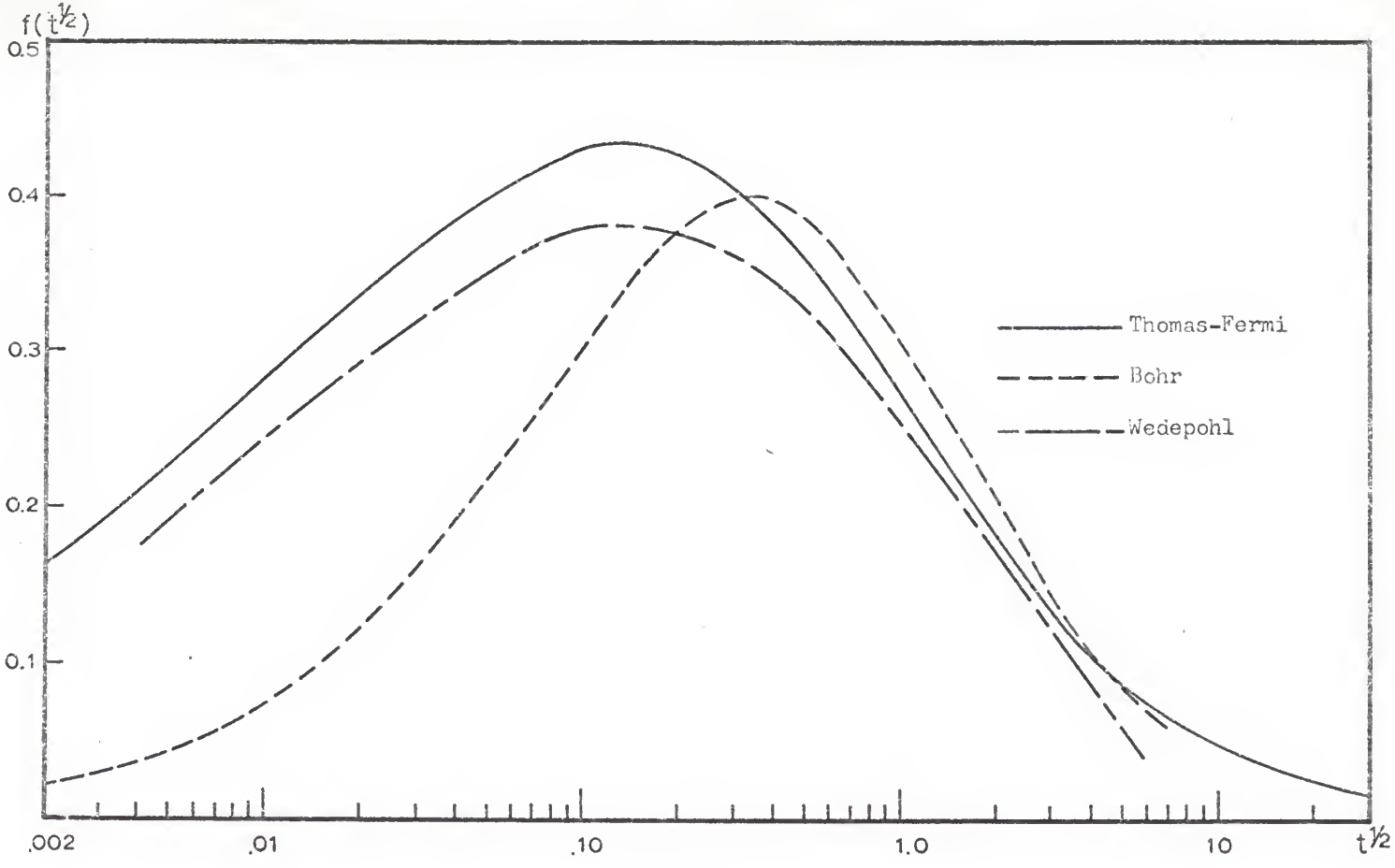

FIGURE 1

Reduced cross section, $f(t^{1/2})$, verses $t^{1/2}$ for the Thomas-Fermi, Bohr, and Wedepohl potentials. $f(t^{1/2})$ and t are defined in equations (28) and (25).

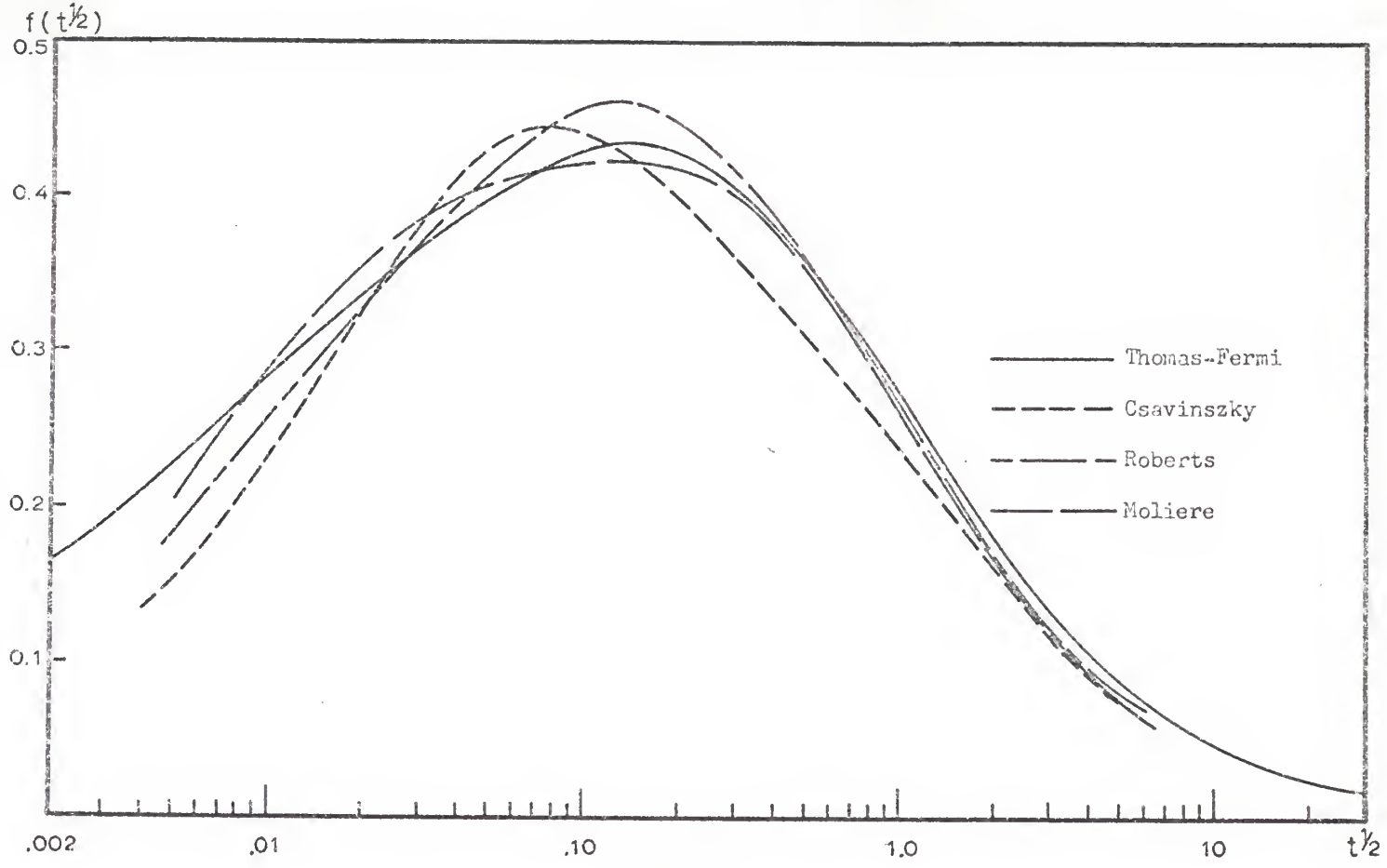

FIGURE 2

Reduced cross section, $f(t^{1/2})$ verses $t^{1/2}$ for the Thomas-Fermi, Csavinszky, Roberts and Moliere potentials. $f(t^{1/2})$ and t are defined in equations (28) and (25).

TABLE XI

Calculated values of $t^{1/2}$ and reduced cross section, $f(t^{1/2})$, for the Bohr potential. t and $f(t^{1/2})$ are defined in equations (25) and (28). The number in parentheses after an entry is the power of 10 to be multiplied by it.

$t^{1/2}$	$f(t^{1/2})$	$t^{1/2}$	$f(t^{1/2})$
0.26505(-3)	0.43366(-2)	0.11354(1)	0.2947
0.35386(-3)	0.48849(-2)	0.14553(1)	0.25376
0.47195(-3)	0.72839(-2)	0.19745(1)	0.20960
0.62316(-3)	0.86247(-2)	0.29582(1)	0.15735
0.84682(-3)	0.11082(-1)	0.30756(1)	0.13914
0.11380(-2)	0.13851(-1)	0.31693(1)	0.13579
0.15524(-2)	0.18191(-1)	0.32683(1)	0.13190
0.20865(-2)	0.23850(-1)	0.33732(1)	0.12817
0.28065(-2)	0.29143(-1)	0.34843(1)	0.12442
0.38242(-2)	0.37415(-1)	0.36024(1)	0.12074
0.51798(-2)	0.46777(-1)	0.37278(1)	0.11730
0.70889(-2)	0.59134(-1)	0.38610(1)	0.11338
0.96875(-2)	0.74894(-1)	0.40035(1)	0.10991
0.13234(-1)	0.93379(-1)	0.41548(1)	0.10640
0.18313(-1)	0.11600	0.43169(1)	0.10246
0.25389(-1)	0.14364	0.44905(1)	0.98797(-1)
0.35423(-1)	0.17669	0.46766(1)	0.95167(-1)
0.49825(-1)	0.21471	0.48763(1)	0.91660(-1)
0.70884(-1)	0.25850	0.50904(1)	0.88070(-1)
0.10225	0.30972	0.53209(1)	0.84237(-1)
0.15063	0.35436	0.55697(1)	0.80840(-1)
0.16659	0.35775	0.58363(1)	0.77344(-1)
0.18476	0.37093	0.61242(1)	0.73796(-1)
0.20528	0.38135	0.64331(1)	0.70509(-1)
0.22870	0.38897	0.67644(1)	0.67095(-1)
0.25560	0.39569	0.71192(1)	0.63868(-1)
0.28666	0.40070	0.74958(1)	0.60866(-1)
0.32283	0.40387	0.78925(1)	0.57880(-1)
0.36529	0.40386	0.83063(1)	0.55051(-1)
0.41582	0.40148	0.87305(1)	0.52428(-1)
0.47654	0.39597	0.91557(1)	0.50068(-1)
0.55077	0.38583	0.95676(1)	0.47971(-1)
0.64338	0.37145	0.99492(1)	0.46174(-1)
0.76176	0.35115	0.10279(2)	0.44724(-1)
0.91854	0.32492	0.10536(2)	0.43584(-1)
		0.10700(2)	0.42953(-1)

TABLE XII

Calculated values of $t^{1/2}$ and reduced cross section, $f(t^{1/2})$, for the Csavinszky potential. t and $f(t^{1/2})$ are defined in equations (25) and (28). The number in parentheses after an entry is the power of 10 to be multiplied by it.

$t^{1/2}$	$f(t^{1/2})$	$t^{1/2}$	$f(t^{1/2})$
0.40014(-2)	0.12744	0.10231(1)	0.24482
0.46285(-2)	0.14225	0.13361(1)	0.21740
0.53520(-2)	0.15784	0.18496(1)	0.18543
0.61910(-2)	0.17410	0.28291(1)	0.14423
0.71690(-2)	0.18828	0.29469(1)	0.12909
0.83354(-2)	0.20638	0.30400(1)	0.12453
0.96898(-2)	0.22544	0.31390(1)	0.12173
0.11302(-1)	0.24442	0.32438(1)	0.11810
0.13210(-1)	0.26762	0.33556(1)	0.11542
0.15461(-1)	0.28881	0.34731(1)	0.11245
0.18173(-1)	0.31314	0.35988(1)	0.10911
0.21400(-1)	0.33569	0.37320(1)	0.10605
0.25347(-1)	0.35851	0.38744(1)	0.10274
0.30147(-1)	0.38344	0.40262(1)	0.99644(-1)
0.36058(-1)	0.40404	0.41886(1)	0.96170(-1)
0.43495(-1)	0.42265	0.43630(1)	0.93023(-1)
0.52982(-1)	0.43674	0.45492(1)	0.89930(-1)
0.65449(-1)	0.44552	0.47495(1)	0.86481(-1)
0.82353(-1)	0.44522	0.49651(1)	0.83205(-1)
0.10648	0.44221	0.51971(1)	0.80011(-1)
0.14279	0.43115	0.54469(1)	0.76745(-1)
0.15495	0.41932	0.57162(1)	0.73533(-1)
0.16863	0.40593	0.60062(1)	0.70419(-1)
0.18446	0.39725	0.63181(1)	0.67197(-1)
0.20266	0.39270	0.66539(1)	0.64129(-1)
0.22368	0.38841	0.70128(1)	0.61121(-1)
0.24852	0.37430	0.73958(1)	0.58172(-1)
0.27784	0.36479	0.78004(1)	0.55386(-1)
0.31307	0.35529	0.82233(1)	0.52697(-1)
0.35561	0.34470	0.86584(1)	0.50223(-1)
0.40804	0.33232	0.90954(1)	0.47978(-1)
0.47363	0.31996	0.95205(1)	0.45942(-1)
0.55716	0.30493	0.99157(1)	0.44206(-1)
0.66673	0.28784	0.10259(2)	0.42807(-1)
0.81469	0.26860	0.10526(2)	0.41701(-1)
		0.10697(2)	0.41067(-1)

TABLE XIII

Calculated values of $t^{1/2}$ and reduced cross section, $f(t^{1/2})$, for the Roberts potential. t and $f(t^{1/2})$ are defined in equations (25) and (28). The number in parentheses after an entry is the power of 10 to be multiplied by it.

$t^{1/2}$	$f(t^{1/2})$	$t^{1/2}$	$f(t^{1/2})$
0.46659(-2)	0.16961	0.10516(1)	0.26450
0.52718(-2)	0.21077	0.13571(1)	0.22977
0.59441(-2)	0.20461	0.18597(1)	0.19111
0.67587(-2)	0.21645	0.28247(1)	0.14561
0.76807(-2)	0.22922	0.29407(1)	0.13071
0.87831(-2)	0.24361	0.30328(1)	0.12470
0.10055(-1)	0.25712	0.31310(1)	0.12218
0.11589(-1)	0.26887	0.32346(1)	0.11905
0.13423(-1)	0.28454	0.33449(1)	0.11572
0.15625(-1)	0.30207	0.34617(1)	0.11283
0.18278(-1)	0.32009	0.35856(1)	0.10955
0.21512(-1)	0.33725	0.37180(1)	0.10576
0.25510(-1)	0.35324	0.38597(1)	0.10269
0.30524(-1)	0.37272	0.40102(1)	0.99352(-1)
0.36826(-1)	0.39038	0.41721(1)	0.96115(-1)
0.44968(-1)	0.40745	0.43446(1)	0.92842(-1)
0.55617(-1)	0.42458	0.45305(1)	0.89477(-1)
0.69884(-1)	0.43935	0.47297(1)	0.86301(-1)
0.89537(-1)	0.45293	0.49441(1)	0.82835(-1)
0.11749	0.46658	0.51754(1)	0.79577(-1)
0.15943	0.46126	0.54244(1)	0.76297(-1)
0.17312	0.45188	0.56934(1)	0.72983(-1)
0.18863	0.45294	0.59834(1)	0.69830(-1)
0.20617	0.44936	0.62956(1)	0.66742(-1)
0.22626	0.44320	0.66311(1)	0.63613(-1)
0.24939	0.43794	0.69911(1)	0.60647(-1)
0.27613	0.43113	0.73743(1)	0.57706(-1)
0.30743	0.42114	0.77804(1)	0.54885(-1)
0.34451	0.41127	0.82049(1)	0.52284(-1)
0.38873	0.39842	0.86416(1)	0.49785(-1)
0.44260	0.38313	0.90813(1)	0.47489(-1)
0.50910	0.36647	0.95097(1)	0.45193(-1)
0.59289	0.34623	0.99078(1)	0.43779(-1)
0.70153	0.32305	0.10254(2)	0.42373(-1)
0.84700	0.29545	0.10524(2)	0.41284(-1)
		0.10697(2)	0.40662(-1)

TABLE XIV

Calculated values of $t^{1/2}$ and reduced cross section, $f(t^{1/2})$, for the Moliere potential. t and $f(t^{1/2})$ are defined in equations (25) and (28). The number in parentheses after an entry is the power of 10 to be multiplied by it.

$t^{1/2}$	$f(t^{1/2})$	$t^{1/2}$	$f(t^{1/2})$
0.50620(-2)	0.19824	0.10500(1)	0.26255
0.57047(-2)	0.20738	0.13573(1)	0.22846
0.64298(-2)	0.23236	0.18630(1)	0.19070
0.72395(-2)	0.24518	0.28345(1)	0.14563
0.81906(-2)	0.25908	0.29509(1)	0.12685
0.92757(-2)	0.27140	0.30445(1)	0.12688
0.10561(-1)	0.28836	0.31425(1)	0.12298
0.12027(-1)	0.30467	0.32469(1)	0.11887
0.13767(-1)	0.31883	0.33581(1)	0.11586
0.15812(-1)	0.33564	0.34755(1)	0.11317
0.18246(-1)	0.34782	0.36002(1)	0.10958
0.21210(-1)	0.35850	0.37335(1)	0.10647
0.24851(-1)	0.37014	0.38749(1)	0.10310
0.29376(-1)	0.38266	0.40269(1)	0.99671(-1)
0.35073(-1)	0.39121	0.41889(1)	0.96611(-1)
0.42475(-1)	0.39710	0.43624(1)	0.93253(-1)
0.52308(-1)	0.40430	0.45486(1)	0.89817(-1)
0.65664(-1)	0.41147	0.47490(1)	0.86606(-1)
0.84396(-1)	0.41660	0.49640(1)	0.83308(-1)
0.11174	0.42658	0.51959(1)	0.79979(-1)
0.15328	0.43337	0.54455(1)	0.76836(-1)
0.16707	0.42613	0.57144(1)	0.73456(-1)
0.18256	0.42255	0.60050(1)	0.70273(-1)
0.20028	0.41912	0.63170(1)	0.67250(-1)
0.22059	0.41718	0.66523(1)	0.64064(-1)
0.24394	0.41419	0.70121(1)	0.61037(-1)
0.27102	0.41082	0.73950(1)	0.58160(-1)
0.30259	0.40463	0.77997(1)	0.55334(-1)
0.34001	0.39633	0.82230(1)	0.52693(-1)
0.38472	0.38698	0.86578(1)	0.50226(-1)
0.43890	0.37490	0.90950(1)	0.47947(-1)
0.50571	0.36004	0.95203(1)	0.45929(-1)
0.58983	0.34162	0.99155(1)	0.44193(-1)
0.69877	0.31925	0.10259(2)	0.42790(-1)
0.84469	0.29312	0.10526(2)	0.41708(-1)
		0.10697(2)	0.41079(-1)

TABLE XV

Calculated values of $t^{1/2}$ and reduced cross section, $f(t^{1/2})$, for the Wedepohl potential. t and $f(t^{1/2})$ are defined in equations (25) and (28). The number in parentheses after an entry is the power of 10 to be multiplied by it.

$t^{1/2}$	$f(t^{1/2})$	$t^{1/2}$	$f(t^{1/2})$
0.42207(-2)	0.18346	0.10206(1)	0.25626
0.47131(-2)	0.18381	0.13138(1)	0.22626
0.52849(-2)	0.19662	0.17811(1)	0.19093
0.59342(-2)	0.20748	0.26358(1)	0.14527
0.66836(-2)	0.21773	0.27361(1)	0.12953
0.75541(-2)	0.22188	0.28156(1)	0.12674
0.86110(-2)	0.22919	0.28994(1)	0.12247
0.98524(-2)	0.24151	0.29883(1)	0.11904
0.11324(-1)	0.25354	0.30820(1)	0.11542
0.13085(-1)	0.26290	0.31816(1)	0.11218
0.15243(-1)	0.27155	0.32866(1)	0.10837
0.17903(-1)	0.28502	0.33991(1)	0.10473
0.21175(-1)	0.29565	0.35180(1)	0.10101
0.25335(-1)	0.30791	0.36458(1)	0.97496(-1)
0.30616(-1)	0.32079	0.37813(1)	0.93839(-1)
0.37500(-1)	0.33296	0.39274(1)	0.89745(-1)
0.46633(-1)	0.34621	0.40842(1)	0.85989(-1)
0.59033(-1)	0.35765	0.42530(1)	0.82436(-1)
0.76474(-1)	0.36764	0.44343(1)	0.78669(-1)
0.10194	0.38129	0.46311(1)	0.74410(-1)
0.14089	0.38918	0.48456(1)	0.70554(-1)
0.15385	0.38026	0.50781(1)	0.66970(-1)
0.16852	0.38005	0.53310(1)	0.62995(-1)
0.18533	0.37648	0.56085(1)	0.59118(-1)
0.20477	0.37531	0.59119(1)	0.55348(-1)
0.22714	0.37457	0.62450(1)	0.51552(-1)
0.25319	0.37026	0.66106(1)	0.47864(-1)
0.28394	0.36552	0.70114(1)	0.44247(-1)
0.32046	0.35880	0.74492(1)	0.40796(-1)
0.36455	0.35179	0.79230(1)	0.37554(-1)
0.41810	0.34372	0.84281(1)	0.34451(-1)
0.48433	0.33246	0.89547(1)	0.31670(-1)
0.56799	0.31935	0.94804(1)	0.29234(-1)
0.67627	0.30139	0.99720(1)	0.27202(-1)
0.82058	0.28112	0.10382(2)	0.25600(-1)
		0.10658(2)	0.24658(-1)

V. DISCUSSION AND CONCLUSION

The procedure used in the present calculations was checked by a comparison of the present calculations to those of Everhart et al.[8] We have extended the above mentioned calculations to include small scattering angles.

Values of $\sigma(\theta)$ and $\theta(b)$ were calculated for the Bohr, Moliere, Csavinszky, Roberts, and Wedepohl potentials. Table VIII illustrates the sensitivity of the scattering angle for a wide range of values of impact parameter, b. We note that for $b \approx 1$ Å, the scattering angle from an interaction of a 50 kev oxygen ion with a carbon target atom with the Bohr potential is about 20 times smaller than angles with other potentials considered in this work. For smaller values of b (≈ 0.3 Å) all the potentials predict the same scattering angles within about 10 per cent.

Csavinszky reports that the potential, which he describes in a closed form (equation (19)), is in reasonable agreement with the Thomas-Fermi potential up to intermediate distances. However, the Csavinszky potential has been claimed to have more desirable behavior at large distances. The Firsov form of the interatomic potential was used in all calculations involving the Csavinszky, Roberts, and Wedepohl potentials. The difference in the screening length, as defined by Thomas-Fermi, and that of Firsov differs by less than 4 per cent.

The reduced cross sections, $f(t^{1/2})$, for the different potentials are given in figures 1 and 2 to provide a comparison with the results of the Thomas-Fermi potential obtained by Lindhard et al.[15] It is noted that the reduced cross section for the Moliere potential agrees reasonably well with the Thomas-Fermi values over a wide range of $t^{1/2}$.

The classical calculations are generally valid when Θ is greater than $\Theta^* \approx \lambda/2\pi a$. When the classical results may be in error, $\sigma(\Theta)$ can be calculated with the Born approximation. The two methods complement each other.

The present calculations can be very conveniently used in Monte Carlo calculations of elastic energy loss for ions in amorphous targets. Some preliminary work has already been completed and further investigations are planned.

ACKNOWLEDGMENT

The author wishes to express his sincere gratitude to Dr. Chander P. Bhalla, for his initiation of the project and his valuable guidance throughout the work. The author also expresses gratitude to Glen P. Reese for his valuable assistance, and to Dr. James R. Macdonald for his discussions on Monte Carlo techniques. He is grateful to the staff of the Kansas State University Computing Center. This work was supported by a N.D.E.A. fellowship.

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CLASSICAL CALCULATIONS OF DIFFERENTIAL SCATTERING CROSS SECTIONS FOR VARIOUS SCREENED POTENTIALS

by

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AN ABSTRACT OF A MASTER'S THESIS

submitted in partial fulfillment of the

requirements for the degree

MASTER OF SCIENCE

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1969

ABSTRACT

Several screened potentials are used in the calculation of the differential cross section and the scattering angle as a function of impact parameter. The numerical results of Everhard et al. (for the Bohr potential) are extended for small angles. The reduced differential cross section is presented as a function of the dimensionless variable $t^{1/2}$ for five potentials. These results can be used for any Z_1, Z_2, and energy where the quantum effects are negligible. The calculations were performed on the IBM 360/50 computer at Kansas State University. The basic computer program can be used in the Monte Carlo calculations of elastic energy loss for ions in matter.