Classical Calculation of Differential Cross Section for Scattering from a Coulomb Potential with Exponential Screening*

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The potential energy function considered is $V=(Z_1Z_2e^2/r)\exp(-r/a)$, which approximately represents the potential between two atoms in collision taking into account the screening of the atomic electrons. Here the first factor is the Coulomb potential and the exponential factor contains a screening length a. It is shown first that a classical orbital calculation should give valid results under certain conditions in problems where ions with energies of many thousands of electron volts scatter from atoms. Calculated values of the impact parameters and differential cross sections are presented for all angles of scattering. These quantities are tabulated for a wide range of parameters corresponding to various degrees of screening.

1. VALIDITY OF A CLASSICAL SOLUTION

THE interaction between two atoms during a collision is approximately represented by the potential energy function,

$$V=(Z_1Z_2e^2/r)\exp(-r/a), \tag{1}$$

over a wide range of energies. The first factor is the Coulomb potential energy function between two nuclei of charges Z_1e and Z_2e. The exponential factor takes into account the electron screening, whose extent is measured by the screening length a. Bohr[1] has discussed this potential in some detail and has suggested the expression,

$$a=a_0/[Z_1^{\frac{2}{3}}+Z_2^{\frac{2}{3}}]^{\frac{1}{2}}, \tag{2}$$

for the screening length. Here a_0 is 0.53×10^{-8} cm, the radius of the first orbit in hydrogen. Mott and Massey[2] have pointed out that a classical calculation of differential cross section for scattering is valid when: (a) the deBroglie wavelength λ of the incident particle is negligible compared with any significant dimension of the scattering center, and when (b) the collision is well defined within the limitations of the uncertainty principle.

Condition (a) requires that λ be much smaller than the screening length a, and also much smaller than the collision diameter b, defined by

$$b=Z_1Z_2e^2/(\tfrac{1}{2}mv^2). \tag{3}$$

In this expression m is the reduced mass of the system, and v is the relative velocity of the collision. The length b, which varies inversely with the energy of the collision would be the distance of closest approach in a "head on" collision were there no screening. Since this length is also the diameter of the cross section of backward scattering in the absence of screening, it is a good measure of the size of the scattering center when b/a is small. Bohr[1] has shown for this potential that the second condition, (b), leads to a lower limit on the scattering angle, namely,

$$\theta^*\approx\lambda/2\pi a. \tag{4}$$

For angles greater than this, the classical solution is valid.

By way of illustration, numbers will be put into the above equations for a particular case. For the collision of 50-kev neon ions with argon atoms, one calculates $a=160\times10^{-11}$ cm, $b=78\times10^{-11}$ cm, $\lambda=0.42\times10^{-11}$ cm, and $\theta^*=0.026$ radian, or 0.15°. Thus both conditions for the validity of a classical solution are satisfied at all angles greater than 0.15° in this case. In fact, for most collisions between atoms in the energy range from about a hundred electron volts to hundreds of thousands of electron volts, the classical calculation of differential cross section is valid except at very small angles. Massey and Smith[3] calculated differential cross sections for 72-ev protons on argon targets, and for 110-ev protons on helium targets using classical methods. They used, however, the self-consistent field instead of the screened Coulomb field considered in the calculations presented here.

There has been no general quantum mechanical solution worked out for the potential of Eq. (1). The Born approximation solution for this potential is well known,[1,4] but when the appropriate validity criteria are examined,[1,2,5] the solution for particles heavier than electrons is found to be valid only for angles less than θ^*, or $\lambda/2\pi a$. Since the classical solution is valid for angles greater than this limit, it is seen that the two methods are valid in mutually exclusive angular ranges.

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[1] N. Bohr, Kgl. Danske Videnskab. Selskab, Mat-fys. Medd. **18**, 8 (1948). Paragraphs 1.4, 1.5, 1.6, and 2.1 are particularly pertinent to the discussion here.

[2] N. F. Mott and H. S. W. Massey, *The Theory of Atomic Collisions* (Oxford University Press, London, 1949), second edition, Chap. VII, Secs. 4 and 5.

[3] H. S. W. Massey and R. A. Smith, Proc. Roy. Soc. (London) **A142**, 142 (1933).

[4] See, for example, L. I. Schiff, *Quantum Mechanics* (McGraw-Hill Book Company, Inc., New York, 1949).

[5] Everhart, Stone, and Carbone, Technical Report No. 2 to Office of Ordnance Research, April 20, 1954 (unpublished).

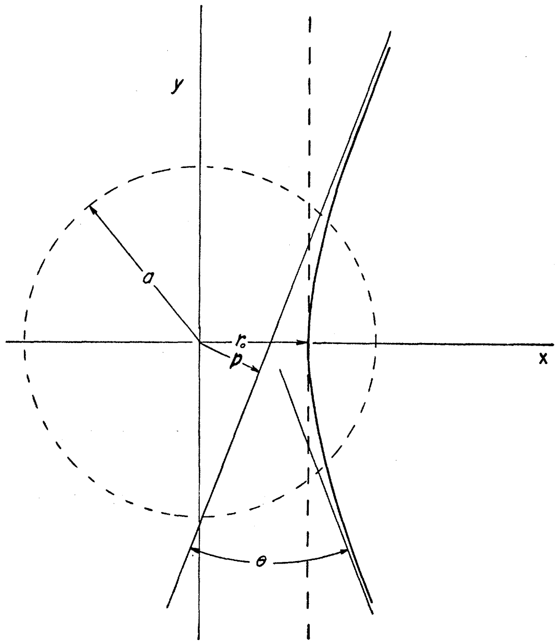

FIG. 1. Orbit of a particle scattered through an angle θ showing the impact parameter p, the distance of closest approach r_0, and the screening length a.

2. TABULATION OF RESULTS

Figure 1 shows a typical orbit in which the impact parameter p, the screening radius a, and the angle of scattering θ are indicated. The distance r_0 shown is the actual closest distance of approach for the orbit.

In any given experimental study, the particles in question and the energy will be known and the corresponding value of b/a is readily calculated from Eqs. (2) and (3). The case $b/a=0$ applies in the limit of higher energies where screening is negligible and here the potential reduces to the Coulomb potential. In this limit the differential cross section is given by the familiar Rutherford formula,

$$\sigma(\theta)=(b^2/16)\csc^4(\theta/2). \tag{5}$$

However, as the energy decreases, b/a increases, which corresponds to more effective screening.

The formulas for the classical calculation of the differential cross section at all angles from a given potential are well known. The integrations for the potential of Eq. (1) must be carried out numerically for each point. The formulas and details of the method of calculation are given in the Appendix to this paper. Of the two numerical procedures presented there, one method is suitable for all angles, and the other, somewhat simpler, is applicable at small angles only.

It is convenient to plot the ratio of the differential cross section $\sigma(\theta)$ to the square of the collision diameter b, since this dimensionless quantity is a function only of angle θ, and the ratio b/a. All calculations are in center-of-mass coordinates. Figure 2 shows $\sigma(\theta)/b^2$ plotted for angles up to 0.6π for eight values of b/a. It shows the general behavior of the screened differential cross section and its relationship to the Rutherford cross section.

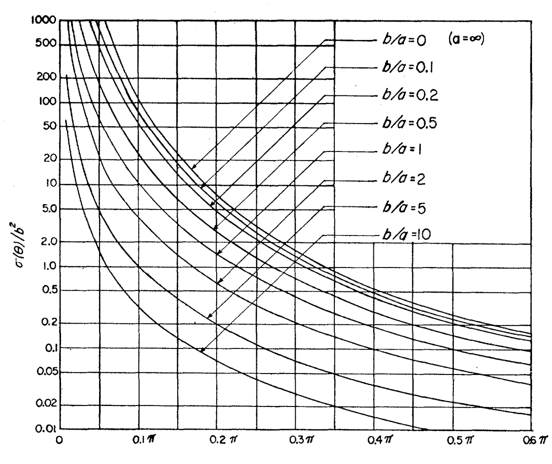

FIG. 2. Differential cross sections $\sigma(\theta)$ for scattering from an exponentially screened Coulomb potential plotted as a function of scattering angle θ in center-of-mass coordinates. Here b is the collision diameter and a is the screening length. For the case $b/a=0$, or $a=\infty$, there is no screening and the curve follows the Rutherford formula. Successively larger values of b/a correspond to more and more effective screening.

Table I gives a complete summary of the numerical results, tabulating actual distance of closest approach, impact parameter, and differential cross section for angles between 0.01π and π and for $b/a=0$, 0.1, 0.2, 0.5, 1, 2, 5, 10. These calculations are particularly useful in interpreting results of experiments in which differential cross sections have been measured for single collisions between atoms at large angles.[6–8]

3. ACKNOWLEDGMENTS

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4. APPENDIX

a. Large-Angle Calculations

The differential cross section for scattering from an arbitrary potential energy function $V(r)$ is calculated classically[2,9] from

$$\sigma(\theta)=-p\,dp/\sin\theta\,d\theta, \tag{6}$$

where

$$\theta=\pi-2\int_{r_0}^{\infty}[r\phi(r)]^{-1}dr, \tag{7}$$

[6] von C. Ramsauer and R. Kollath, Ann. Physik **16**, 570 (1933).
[7] A. G. Rouse, Phys. Rev. **52**, 1238 (1937).
[8] Everhart, Carbone, and Stone, Phys. Rev. **98**, 1045 (1955).
[9] H. S. W. Massey and E. H. S. Burhop, *Electronic and Ionic Impact Phenomena* (Oxford University Press, London, 1952), p. 373.

and

$$\phi(r)=[r^2/p^2-1-r^2V(r)/(\tfrac{1}{2}mv^2p^2)]^{\frac{1}{2}}. \tag{8}$$

Here r_0 is the largest positive root of Eq. (8). Letting $z=a/r$ in the above equations and substituting

$$V(r)=(\tfrac{1}{2}mv^2b/r)\exp(-r/a)$$

from Eqs. (1) and (3) into Eq. (7) there results

$$\theta=\pi-2(p/a)\int_0^{z_0} y^{-\frac{1}{2}}dz, \tag{9}$$

where

$$y=1-(p/a)^2z^2-(b/a)z\exp(-1/z), \tag{10}$$

and z_0 is the root of Eq. (10). The integral of Eq. (9) must be evaluated numerically for each value of p/a and b/a. In this form there is difficulty in maintaining sufficient accuracy at some angles because the second term of Eq. (9) is comparable with π and must then be subtracted from π to find θ. Letting

$$y_0=1-(p/a)^2z^2-(b/a)z\exp(-1/z_0), \tag{11}$$

Eq. (9) can be put into another form:

$$\theta=\pi-2(p/a)\left[\int_0^{z_0} y_0^{-\frac{1}{2}}dz-\int_0^{z_0}(y_0^{-\frac{1}{2}}-y^{-\frac{1}{2}})dz\right], \tag{12}$$

in which the first integral is readily evaluated analytically. The π cancels and the result is

$$\theta=2\cot^{-1}\left[\frac{2p/b}{\exp(-1/z_0)}\right]+\frac{2p}{a}\int_0^{z_0}(y_0^{-\frac{1}{2}}-y^{-\frac{1}{2}})dz. \tag{13}$$

In this form the numerical evaluation of the remaining integral by Simpson's rule yields a small quantity which is added to the first term and accuracy is maintained. There is an infinity in the integrand at $z=z_0$ which varies as $(z_0-z)^{-\frac{1}{2}}$ and has to be handled separately. Three place accuracy was maintained in the calculation of θ as a function of p/b.

The calculation of $dp/d\theta$ needed for Eq. (6) was done graphically using large scale plots of p/b *vs* θ on both linear and logarithmic scales. A careful plot of the resulting values of $dp/d\theta$ *vs* θ indicates that our values of this quantity for each point are accurate to within 2 percent. The final cross sections, calculated from Eq. (6) are thus correct to within 2 percent also. This should be sufficiently accurate for comparison with experimental data since the cross sections are rapidly varying functions of angle.

b. Small-Angle Calculations

At small angles there is a simpler method based on a calculation of the sideways impulse during a collision. As shown by the dotted line in Fig. 1, the actual path of the particle is approximated by a straight line $x=r_0$ parallel to the y-axis along which the particle moves with constant velocity v. Although the dotted line is

TABLE I. Distances of closest approach r_0, impact parameter p, and differential cross sections $\sigma(\theta)$ calculated classically for scattering from an exponentially screened Coulomb potential. Here a is the screening length and b is the collision diameter. Angles θ are in center-of-mass coordinates.

	$b/a=0$ ($a=\infty$)			$b/a=0.1$		
θ	r_0/b	p/b	$\sigma(\theta)/b^2$	r_0/b	p/b	$\sigma(\theta)/b^2$
0.01π	32.3	31.8	1.03×10^6	14.3	14.2	1.02×10^5
0.02π	16.4	15.9	6.42×10^4	9.85	9.65	1.47×10^4
0.03π	11.1	10.6	1.27×10^4	7.63	7.39	4.27×10^3
0.04π	8.46	7.95	4.02×10^3	6.28	6.00	1.71×10^3
0.06π	5.81	5.29	7.97×10^2	4.69	4.37	4.45×10^2
0.08π	4.49	3.96	2.53×10^2	3.78	3.42	1.62×10^2
0.10π	3.70	3.16	1.04×10^2	3.19	2.81	7.4×10^1
0.15π	2.64	2.08	2.11×10^1	2.35	1.91	1.67×10^1
0.20π	2.12	1.54	6.85×10^0	1.90	1.43	5.7×10^0
0.30π	1.60	0.981	1.47×10^0	1.45	0.924	1.28×10^0
0.40π	1.35	0.688	5.23×10^{-1}	1.24	0.651	4.64×10^{-1}
0.50π	1.21	0.500	2.50×10^{-1}	1.10	0.474	2.23×10^{-1}
0.75π	1.04	0.207	8.57×10^{-2}	0.961	0.197	7.7×10^{-2}
π	1.00	0	6.25×10^{-2}	0.913	0	5.65×10^{-2}
	$b/a=0.2$			$b/a=0.5$		
θ	r_0/b	p/b	$\sigma(\theta)/b^2$	r_0/b	p/b	$\sigma(\theta)/b^2$
0.01π	9.59	9.51	3.63×10^4	5.26	5.22	8.1×10^3
0.02π	7.11	6.99	6.3×10^3	4.16	4.10	1.70×10^3
0.03π	5.77	5.62	2.01×10^3	3.56	3.48	6.1×10^2
0.04π	4.94	4.75	8.8×10^2	3.14	3.04	2.91×10^2
0.06π	3.87	3.63	2.62×10^2	2.60	2.46	9.8×10^1
0.08π	3.19	2.92	1.06×10^2	2.22	2.06	4.32×10^1
0.10π	2.74	2.44	5.1×10^1	1.99	1.80	2.26×10^1
0.15π	2.09	1.73	1.29×10^1	1.59	1.35	6.5×10^0
0.20π	1.73	1.32	4.65×10^0	1.35	1.07	2.57×10^0
0.30π	1.34	0.865	1.09×10^0	1.08	0.729	6.9×10^{-1}
0.40π	1.13	0.615	4.06×10^{-1}	0.931	0.529	2.78×10^{-1}
0.50π	1.02	0.450	1.99×10^{-1}	0.839	0.391	1.43×10^{-1}
0.75π	0.878	0.187	7.0×10^{-2}	0.738	0.166	5.4×10^{-2}
π	0.845	0	5.14×10^{-2}	0.703	0	4.01×10^{-2}
	$b/a=1$			$b/a=2$		
θ	r_0/b	p/b	$\sigma(\theta)/b^2$	r_0/b	p/b	$\sigma(\theta)/b^2$
0.01π	3.22	3.20	2.80×10^3	1.91	1.90	8.5×10^2
0.02π	2.63	2.59	5.7×10^2	1.61	1.59	1.86×10^2
0.03π	2.30	2.25	2.15×10^2	1.43	1.40	7.2×10^1
0.04π	2.08	2.02	1.06×10^2	1.31	1.28	3.61×10^1
0.06π	1.78	1.70	3.82×10^1	1.15	1.10	1.34×10^1
0.08π	1.58	1.47	1.81×10^1	1.04	0.975	6.6×10^0
0.10π	1.41	1.29	9.8×10^0	0.957	0.880	3.76×10^0
0.15π	1.16	1.00	3.13×10^0	0.817	0.712	1.34×10^0
0.20π	1.03	0.828	1.37×10^0	0.723	0.595	6.3×10^{-1}
0.30π	0.844	0.588	4.25×10^{-1}	0.610	0.438	2.14×10^{-1}
0.40π	0.736	0.435	1.83×10^{-1}	0.542	0.332	1.00×10^{-1}
0.50π	0.671	0.326	9.8×10^{-2}	0.497	0.252	5.6×10^{-2}
0.75π	0.593	0.140	3.84×10^{-2}	0.440	0.110	2.36×10^{-2}
π	0.567	0	2.90×10^{-2}	0.426	0	1.83×10^{-2}
	$b/a=5$			$b/a=10$		
θ	r_0/b	p/b	$\sigma(\theta)/b^2$	r_0/b	p/b	$\sigma(\theta)/b^2$
0.01π	0.919	0.914	1.66×10^2	0.523	0.520	4.75×10^1
0.02π	0.798	0.789	3.63×10^1	0.460	0.455	1.06×10^1
0.03π	0.727	0.715	1.50×10^1	0.425	0.418	4.36×10^0
0.04π	0.679	0.662	7.8×10^0	0.398	0.389	2.31×10^0
0.06π	0.610	0.587	3.13×10^0	0.363	0.350	9.5×10^{-1}
0.08π	0.561	0.531	1.64×10^0	0.338	0.321	5.1×10^{-1}
0.10π	0.525	0.487	9.7×10^{-1}	0.319	0.299	3.15×10^{-1}
0.15π	0.465	0.411	3.80×10^{-1}	0.284	0.254	1.28×10^{-1}
0.20π	0.420	0.352	1.90×10^{-1}	0.263	0.222	6.8×10^{-2}
0.30π	0.360	0.267	7.1×10^{-2}	0.230	0.173	2.74×10^{-2}
0.40π	0.329	0.209	3.58×10^{-2}	0.211	0.138	1.48×10^{-2}
0.50π	0.305	0.162	2.17×10^{-2}	0.198	0.109	9.2×10^{-3}
0.75π	0.273	0.073	1.02×10^{-2}	0.180	0.050	4.74×10^{-3}
π	0.265	0	8.14×10^{-3}	0.175	0	3.84×10^{-3}

not close to the particular orbit shown in Fig. 1, it would lie close to the actual path of the particle if the figure were drawn for a case where the scattering angle θ was small. The x-component of the impulse along this path is assumed to be approximately the same as it would be along the actual path. This impulse over half the path is

$$mv_x=\int_0^\infty (-dV/dr)(x/r)dt, \tag{14}$$

where x/r is the cosine of the angle between the radial force $-dV/dr$ and the x-axis, and v_x is the final x-velocity. The integrand becomes a function of time alone when it is assumed that

$$x=r_0 \quad \text{and} \quad r=(r_0^2+v^2t^2)^{\frac{1}{2}}, \tag{15}$$

in accordance with the approximate path assumed above. An example of calculation of impulse in this way has been given by Bohr.[10] The ratio of the final x-momentum to the initial momentum mv is then half the angle of scattering. Thus

$$\theta/2=mv_x/mv. \tag{16}$$

For the potential energy function of Eq. (1), when one uses Eqs. (3), (14), (15), and (16), the integral is found to be

$$\frac{\theta a}{b}=\int_1^\infty \frac{(a/r_0+u)\exp(-ur_0/a)du}{u^2(u^2-1)^{\frac{1}{2}}}, \tag{17}$$

where $u=(1+v^2t^2/r_0^2)^{\frac{1}{2}}$. Upon integrating the first term in the integrand of Eq. (17) by parts twice and the second term by parts once, the infinities at $u=1$ disappear and there is some cancellation. A simpler form results:

$$\theta a/b=(r_0/a)\int_1^\infty (u^2-1)^{\frac{1}{2}}\exp(-ur_0/a)du. \tag{18}$$

By letting $u=1/w$, an equivalent integral, with limits on w of zero to unity, can be obtained which is suitable for numerical integration. Although applicable only at small angles, this method has the advantage that $\theta a/b$ is a function only of r_0/a. Thus a single set of numerical integrations finds this function for all values of b/a.

Although r_0 is nearly equal to the impact parameter p at small angles, it is considerably more accurate not to assume them equal and to calculate p/r_0 for each value of b/a. By using Eq. (10) with $z_0=a/r_0$, the relationship is seen to be

$$p/r_0=[1-(b/r_0)\exp(-r_0/a)]^{\frac{1}{2}}. \tag{19}$$

By using Eqs. (18) and (19), it is possible to plot curves of p/b as a function of θ for each value of b/a. These curves agree with those obtained from the large-angle calculations of Eq. (13) very well at small angles, departing by no more than 1 percent at angles as large as 0.1π. The rest of the procedure, obtaining $dp/d\theta$ and calculating the differential cross section, is the same as has been described in the large-angle calculations.

[10] See reference 1, p. 9.