

where F is the ordinary hypergeometric function of four variables. Although the exchange integral (14) is easily evaluated for a particular value of n , we have been unable to obtain a simple, closed expression for n generally. Table II contains the results of energy calculations for the $1s3d$ and $1s4d$ configurations of He I, obtained with the use of the hydrogenic energy integrals. The agreement with experiment is excellent. Indeed, the calculated $1s4d$ energies are slightly below the experimental values, which is due to the departure of the hydrogenic functions from exact orthogonality. It may be noted that the parameter $\mu(4d)$, which would possess the value 2 if the functions were exactly orthogonal, departs from that figure only in the fifth decimal.

TABLE II. Results for He I $1s3d$ and $1s4d$.

	$1s3d$	$1s4d$		$1s3d$	$1s4d$
$\mu(3^3D)$	2.00000	2.00003	$\mu(3^1D)$	2.00000	2.00002
$W(3^3D)_{\text{cal}}$	4.11114	4.06261	$W(3^1D)_{\text{cal}}$	4.11109	4.06257
$W(3^3D)_{\text{exp}}$	4.11126	4.06257	$W(3^1D)_{\text{exp}}$	4.11123	4.06255

The wave functions derived in this investigation have been utilized by one of us⁵ to calculate transition probabilities for a number of lines of He I.

It is a pleasure to record our thanks to Dr. P. M. Morse for his interest and guidance in this problem, and to Dr. D. H. Menzel for many valuable discussions of the properties of hypergeometric functions.

⁵ Goldberg, *Astrophys. J.*, in press.

Numerical Calculations of the Reflection of Electrons by Metals

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The specular reflection of electrons by metallic surfaces is considered. It is assumed that the potential energy of an electron is constant ($= -V_0$) in the interior of the metal, and account is taken of the image force acting on an electron outside the metal (Nordheim's problem). The reflection coefficient R is computed for the range of values of V_0 which is of interest in connection with real metals, and for the range of values of energy of the electrons in which R has appreciable values. In the Appendix there are given some values of the function $\Gamma'(iy)/\Gamma(iy)$, for real values of y , which were computed incidentally.

1. INTRODUCTION

THE chief purpose of this article is to give the results of some numerical calculations of the reflection coefficient for a beam of electrons impinging on the plane face of a thick metallic body. We make use of the crude and simple assumption that the potential energy of an electron is constant in the interior of the metal, and we take account of the electrostatic image force acting on an electron outside the metal. Most of the analytical features of the problem have been discussed in an article by Nordheim;¹

but his work was not carried to the point of obtaining numerical results, such as are given here.

2. GENERAL FORMULA FOR THE REFLECTION COEFFICIENT

We employ a rectangular coordinate system, and assume that the metallic body occupies the space to the left of the plane $x=0$. The potential energy of an electron at the point (x, y, z) is assumed to be given by the equations:

$$V(x, y, z) = -V_0, \quad x \leq x_0, \\ = -e^2/4x, \quad x \geq x_0.$$

¹L. Nordheim, *Proc. Roy. Soc. London* **A121**, 626-639 (1928). Unfortunately, Nordheim's article contains a number of typographical errors, which render the formulae

unreliable. All formulae used in the present work have been derived independently.

Here ϵ denotes the absolute value of the electronic charge; and x_0 is determined by the equation $V_0 = \epsilon^2/(4x_0)$, so that $V(x, y, z)$ is continuous. V_0 is a positive parameter, the value of which is to be selected in accordance with the metal under consideration.

We confine our attention to electrons having total energy E . One solution of the wave equation,

$$\nabla^2\psi + k^2(E - V)\psi = 0, \quad k^2 \doteq 8\pi^2m/h^2,$$

for these electrons is represented by the equations:

$$\begin{aligned} \psi = & B_1 \exp \{ ik[-x(E_x + V_0)^{\frac{1}{2}} \\ & + (p_y y + p_z z)/(2m)^{\frac{1}{2}}] \}, \quad x \leq x_0, \\ = & [A_2 W_{\lambda, \frac{1}{2}}(\xi) + B_2 W_{-\lambda, \frac{1}{2}}(-\xi)] \\ & \times \exp [ik(p_y y + p_z z)/(2m)^{\frac{1}{2}}], \quad x \geq x_0. \end{aligned} \quad (1)$$

Here p_y and p_z denote arbitrary constants, and the symbols E_x , ξ , and λ , are defined by the equations

$$E_x = E - (p_y^2 + p_z^2)/(2m),$$

$$\xi = 2ikx E_x^{\frac{1}{2}},$$

$$\lambda = -ik\epsilon^2/(8E_x^{\frac{3}{2}}).$$

The symbols $W_{\lambda, \frac{1}{2}}(\xi)$ and $W_{-\lambda, \frac{1}{2}}(-\xi)$ denote the usual confluent hypergeometric functions.² The three constants B_1 , A_2 , and B_2 , are subject to the two relations,

$$\begin{aligned} B_1 \exp [-ikx_0(E_x + V_0)^{\frac{1}{2}}] \\ = & A_2 W_{\lambda, \frac{1}{2}}(2ikx_0 E_x^{\frac{1}{2}}) + B_2 W_{-\lambda, \frac{1}{2}}(-2ikx_0 E_x^{\frac{1}{2}}), \\ - & (E_x + V_0)^{\frac{1}{2}} B_1 \exp [-ikx_0(E_x + V_0)^{\frac{1}{2}}] \\ = & 2E_x^{\frac{1}{2}} [A_2 W'_{\lambda, \frac{1}{2}}(2ikx_0 E_x^{\frac{1}{2}}) \\ & - B_2 W'_{-\lambda, \frac{1}{2}}(-2ikx_0 E_x^{\frac{1}{2}})], \end{aligned} \quad (2)$$

which are consequences of the requirement that the functions ψ , $\partial\psi/\partial x$, $\partial\psi/\partial y$, and $\partial\psi/\partial z$, be continuous at every point of the plane $x = x_0$.

The physical significance of the solution (1) can be determined easily with the aid of the following asymptotic representations of the functions $W_{\pm\lambda, \frac{1}{2}}(\pm\xi)$:

$$W_{\pm\lambda, \frac{1}{2}}(\pm\xi) \sim e^{\mp\frac{1}{2}\xi} (\pm\xi)^{\pm\lambda} \left[1 + \frac{\sum_{n=1}^{\infty} \frac{[\frac{1}{4} - (\pm\lambda - \frac{1}{2})^2][\frac{1}{4} - (\pm\lambda - \frac{3}{2})^2] \cdots [\frac{1}{4} - (\pm\lambda - n + \frac{1}{2})^2]}{n!(\pm\xi)^n} \right]. \quad (3)$$

It is found that the wave function

$$A_2 W_{\lambda, \frac{1}{2}}(\xi) \exp [ik(p_y y + p_z z)/(2m)^{\frac{1}{2}}]$$

represents an incident beam of electrons moving toward the surface of the metal, and that the wave function

$$B_2 W_{-\lambda, \frac{1}{2}}(-\xi) \exp [ik(p_y y + p_z z)/(2m)^{\frac{1}{2}}]$$

represents a reflected beam of electrons moving away from the surface. (For $x < x_0$ our wave

function ψ represents a transmitted beam of electrons moving toward the left from the plane $x = x_0$.) It is clear that E_x is the total energy of an electron diminished by the kinetic energy associated with the component of momentum parallel to the surface of the metal.

The intensities of the incident and reflected beams are proportional to $|A_2|^2$ and $|B_2|^2$, respectively; and hence the reflection coefficient is $R = |B_2/A_2|^2$. By Eqs. (2), we have the following formula for the reflection coefficient:

$$R = \left| \frac{2E_x^{\frac{1}{2}} W'_{\lambda, \frac{1}{2}}(2ikx_0 E_x^{\frac{1}{2}}) + (E_x + V_0)^{\frac{1}{2}} W_{\lambda, \frac{1}{2}}(2ikx_0 E_x^{\frac{1}{2}})}{-2E_x^{\frac{1}{2}} W'_{-\lambda, \frac{1}{2}}(-2ikx_0 E_x^{\frac{1}{2}}) + (E_x + V_0)^{\frac{1}{2}} W_{-\lambda, \frac{1}{2}}(-2ikx_0 E_x^{\frac{1}{2}})} \right|^2. \quad (4)$$

3. THE LIMIT OF R AS E_x APPROACHES ZERO

The limit of R as E_x approaches zero is of interest, because this is the condition of grazing incidence, and also because this is the condition

under which R has its greatest value. In order to

² Demonstrations of the properties of the confluent hypergeometric functions which we use are to be found in: E. T. Whittaker and G. N. Watson, *Modern Analysis* (Cambridge University Press, 4th ed., 1927), Chapter XVI.

calculate the limit, we go back to the equation

$$\frac{\partial^2 \psi}{\partial x^2} + k^2 \left[E_x + \frac{\epsilon^2}{4x} \right] \psi = 0,$$

set E_x equal to zero, and obtain a reflection coefficient R_0 by means of a calculation which is independent of the above, but is parallel to it. We find that R_0 is given by the formula

$$R_0 = \frac{|f_1'(x_0) + ikV_0^{1/2}f_1(x_0)|^2}{|f_2'(x_0) + ikV_0^{1/2}f_2(x_0)|^2}, \quad (5)$$

where

$$f_1(x) = x^{1/2} [J_1(k\epsilon x^{1/2}) - iY_1(k\epsilon x^{1/2})],$$

$$f_2(x) = x^{1/2} [J_1(k\epsilon x^{1/2}) + iY_1(k\epsilon x^{1/2})].$$

Here J_1 and Y_1 denote the usual Bessel functions.

It can be proved that R_0 is in fact equal to $\lim_{E_x \rightarrow 0} R$. Since the proof is rather long, when it is given completely and rigorously, it will be omitted.³

4. NUMERICAL CALCULATIONS AND RESULTS

Our numerical results are given graphically, in a self-explanatory form, by the curves of Figs. 1 and 2. Only a few remarks about the calculations are necessary.

The values of the confluent hypergeometric functions and their derivatives, which were required, were computed by means of the formula

$$W_{\lambda, 1}(\xi) = \frac{1}{\Gamma(1-\lambda)} e^{-\frac{1}{2}\xi}$$

$$+ e^{-\frac{1}{2}\xi} \sum_{n=1}^{\infty} \left[\frac{\Gamma'(n-\lambda)}{\Gamma(n-\lambda)} - \frac{\Gamma'(n+1)}{\Gamma(n+1)} - \frac{\Gamma'(n)}{\Gamma(n)} \right]$$

$$\times \frac{\Gamma(n-\lambda)\xi^n}{n!(n-1)!\Gamma(-\lambda)\Gamma(1-\lambda)}$$

$$+ e^{-\frac{1}{2}\xi} \log \xi \sum_{n=1}^{\infty} \frac{\Gamma(n-\lambda)}{n!(n-1)!\Gamma(-\lambda)\Gamma(1-\lambda)} \xi^n,$$

³ The author merely established the equality $R_0 = \lim_{E_x \rightarrow 0} R$ on the basis of general function-theoretic considerations. A paper by W. C. Taylor (J. Math. and Phys. 18, 34-49 (1939)), which has just appeared, contains formulae, relating specifically to the confluent hypergeometric functions, from which the equality can be inferred at once.

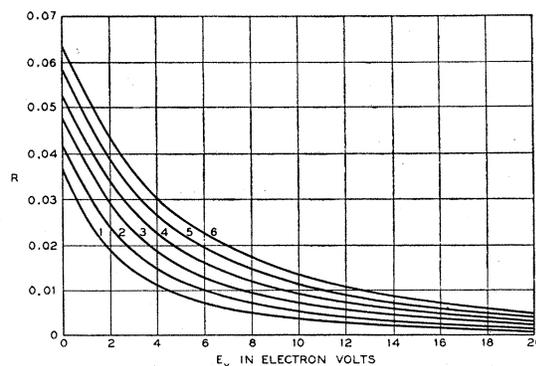


FIG. 1. Reflection coefficient R as a function of E_x . (Curves 1, 2, 3, 4, 5, 6 are for V_0 equal to 10, 12, 14, 16, 18, 20 electron volts, respectively.)

and the formula which is obtained by applying the ordinary formal operations of differentiation with respect to ξ to this.⁴ This formula was obtained by a process which is indicated, but not carried out completely, by Whittaker and Watson.⁵ In order to make use of these formulae (with the aid of the available tables, and of the equations $\Gamma(z+1) = z\Gamma(z)$ and $\Gamma'(z+1)/\Gamma(z+1) = \Gamma'(z)/\Gamma(z) + 1/z$), it was necessary first to compute a short table of values of $\Gamma'(z)/\Gamma(z)$ for pure imaginary values of z . This was done by means of the relation

$$\frac{\Gamma'(z)}{\Gamma(z)} = -\gamma - \frac{1}{z} + \sum_{n=1}^N (-1)^{n+1} \zeta(n+1) z^n$$

$$+ (-1)^N z^{N+1} \sum_{n=1}^{\infty} \frac{1}{n^{N+1}(n+z)},$$

using a value of N large enough so that the series

$$\sum_{n=1}^{\infty} \frac{1}{n^{N+1}(n+z)}$$

converged with satisfactory rapidity. (γ denotes Euler's constant, and ζ denotes the Riemann zeta-function.)

The substantial accuracy of the complicated numerical calculations was strongly indicated by the agreement between the values of the reflection coefficient, for $E_x = 0$, calculated directly by

⁴ For imaginary values of λ and ξ , $W_{-\lambda, 1}(-\xi)$ is merely the conjugate of $W_{\lambda, 1}(\xi)$.

⁵ See also Nordheim's paper.

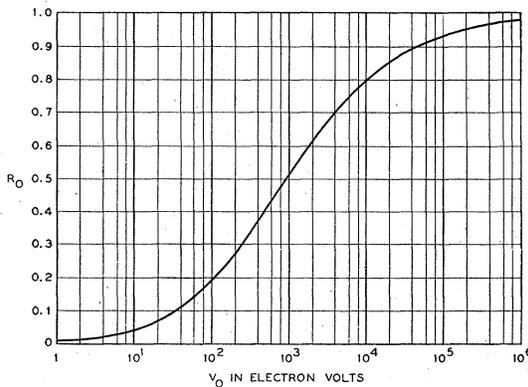


FIG. 2. $R_0 (= \lim_{E_x \rightarrow 0} R)$ as a function of V_0 .

means of Eq. (5), and the values obtained by extrapolating the curves calculated by means of Eq. (4) to the line $E_x = 0$. Actually, it is estimated that the calculated values of R are correct to better than one-tenth percent in neighborhood of $E_x = 1$ electron volt, and to about one percent in the neighborhood of $E_x = 20$ electron volts.

The asymptotic formulae (3) are of no value in computing R for such values of E_x as those shown in Fig. 1, but they do enable us to determine the asymptotic behavior of R for very large values of E_x . This behavior is represented by the formula

$$R \sim \frac{V_0^4}{4e^4 k^2 E_x^3}.$$

The reflection coefficient R_0 given by Eq. (5) is a function of the single variable V_0 . The values of V_0 appropriate to the cases of real metals lie between ten and twenty electron volts. However, in order to show the nature of the function R_0 more completely, we have plotted it, in Fig. 2, for a considerably greater range of values of V_0 . It is easily shown, by means of the known representations of the Bessel functions for large and small values of their arguments, respectively, that when V_0 is

small we have, approximately,

$$R_0 = \frac{V_0}{4k^2 e^4},$$

and that when V_0 is large we have

$$R_0 \sim 1 - \frac{\pi k e^2}{V_0^{\frac{1}{2}}}.$$

In conclusion, we call attention to the fact that if we had left the image force out of account, that is, if we had assumed the potential energy to be

$$V(x, y, z) = -V_0, \quad x < 0, \\ = 0, \quad x > 0,$$

the reflection coefficient would have been given by the equation

$$R = \frac{|(E_x + V_0)^{\frac{1}{2}} - E_x^{\frac{1}{2}}|^2}{|(E_x + V_0)^{\frac{1}{2}} + E_x^{\frac{1}{2}}|^2}.$$

For the values of V_0 and E_x which are of interest, this formula gives values of R which are greater than those given by (4) by a factor which is of the order of ten. Hence, when actual values of R are required, we can by no means neglect the effect of the image force.

APPENDIX

The values of $\Gamma'(iy)/\Gamma(iy)$, for real values of y , which we have computed incidentally, may conceivably be useful in other work. Hence, we record them here. The eight decimal places shown are believed to be quite correct.

y	$\Gamma'(iy)/\Gamma(iy)$
0.1	-0.56529779 + i(10.16342116)
0.2	-0.53073041 + i(5.32064142)
0.3	-0.47675489 + i(3.79986145)
0.4	-0.40786794 + i(3.09770369)
0.5	-0.32888636 + i(2.71268857)
0.6	-0.24419658 + i(2.47826542)
0.7	-0.15733613 + i(2.32420192)
0.8	-0.07088340 + i(2.21654578)
0.9	+0.013452015 + i(2.13738747)
1.0	+0.09465032 + i(2.07667405)