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THE PENETRATION OF A POTENTIAL BARRIER BY ELECTRONS

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Abstract

A potential barrier of the kind studied by Fowler and others may be represented by the analytic function V (Eq. (1)). The Schrödinger equation associated to this potential is soluble in terms of hypergeometric functions, and the coefficient of reflection for electrons approaching the barrier with energy W is calculable (Eq. (15)). The approximate formula,

$$1-\rho=\exp\{-\int\frac{4\pi}{h}(2m(V-W))^{1/2}dx\}$$

is shown to agree very well with the exact formula when the width of the barrier is great compared to the de Broglie wave-length of the incident electron, and $W<V_{max}$.

The "failure" of the law of conservation of energy in quantum dynamics, as evidenced by the penetration of an electron through a region of space in which its potential energy is greater than its total energy, has been advanced as the explanation of several phenomena. Gamow,[1] Gurney and Condon,[2] and others have discussed it in relation to the Geiger-Nuttall law of the radioactive decay constants; Fowler and Nordheim[3] in its relation to the lowering of the thermionic work-function by surface impurities, and to the emission of electrons from cold metals under the influence of strong fields.

The mathematical discussions in these papers have all been based either on a potential function which has discontinuous derivatives, or else on approximate treatments involving asymptotic (i.e., divergent) series. It is therefore of some interest to note that there is an analytic function which represents some of the types of potential barriers which have been discussed and whose associated Schrödinger equation is soluble. This function is

$$V(x) = -A\xi/(1-\xi) - B\xi/(1-\xi)^2, \qquad \xi = -\exp(2\pi x/l), \tag{1}$$

[1] G. Gamow, Zeits. f. Physik **51**, 204 (1928).

[2] R. W. Gurney and E. U. Condon, Phys. Rev. **33**, 127 (1929).

[3] R. H. Fowler, Proc. Roy. Soc. **A122**, 36 (1929), **A117**, 549 (1927). L. Nordheim, Zeits. f. Physik **46**, 833 (1928).

in which x is the cartesian coordinate, and A, B, and l are constants. The graphs of this function for various values of A and B are shown in Fig. 1. It is seen to approach zero for large negative values of x and a constant value

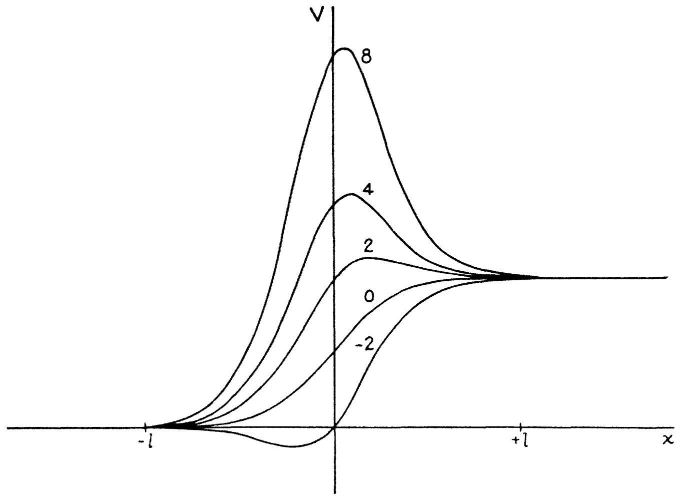

Fig. 1. Graphs of the function $V(x)$. The numbers on the curves are the values of B/A.

A for large positive values. The width of the transition region is, practically speaking, $2l$. When $|B|$ is greater than $|A|$ it possesses an extremum at

$$x_m = \frac{l}{2\pi} \log\ [(B + A)/(B - A)],$$

whose height is

$$V(x_m) = V_m = (A + B)^2/4B. \tag{2}$$

In the following, it will be assumed that $B \geqq 0$ so that the extremum is a maximum, when it exists at all.

The wave equation governing the dynamical problem of an electron moving under the action of this potential is

$$\frac{d^2u}{dx^2} + \frac{8\pi^2 m}{h^2}\{A\xi/(1 - \xi) + B\xi/(1 - \xi)^2 + W\}u = 0 \tag{3}$$

or if differentiation with respect to ξ be indicated by an accent

$$\xi^2 u'' + \xi u' + \frac{2ml^2}{h^2}\{A\xi/(1 - \xi) + B\xi/(1 - \xi)^2 + W\}u = 0. \tag{4}$$

This equation[4] is of the hypergeometric type, and its solutions may therefore be written down at once in terms of the hypergeometric series:[5]

[4] Special cases ($A = 0$, and $B = 0$) of this equation were discussed in the Colloquium at Pasadena by Professor P. Epstein in 1925, the occasion being the work of Epstein and Robertson on the reflection of radio waves by the Heaviside layer.

[5] F. Klein, Ueber die hypergeometrischen Reihen, (Göttingen, 1894) pp. 3–7. A. R. Forsythe, Treatise on Differential Equations, (2[d], one vol. ed.) (New York, 1888) p. 185.

$$F(a,b,c,y) = 1 + \frac{a\cdot b}{1\cdot c}y + \frac{a(a+1)\cdot b(b+1)}{1\cdot 2\cdot c(c+1)}y^2 + \cdots . \tag{5}$$

Before proceeding to study the exact solutions, it will be well to consider their asymptotic behavior for very large positive and negative values of x. In both cases, the potential is practically constant and therefore the solutions should be monochromatic de Broglie waves to a first approximation. For large negative values of x the wave-length will be $\lambda = h/(2mW)^{1/2}$, for large positive values, $\lambda' = h/(2m(W-A))^{1/2}$. It may be assumed that $W \geqq A$, since the interest in the other case is not very great. The solution may be specified even more precisely if we confine ourselves to the case in which the electrons are incident on the barrier from $x = -\infty$. Then there will be a single (transmitted) wave

$$\exp(2\pi i x/\lambda') = (-\xi)^{i\beta}, \quad \beta = l/\lambda' \tag{6}$$

for large positive values of x, and two waves (incident and reflected) for large negative values of x:

$$a_1 \exp(2\pi i x/\lambda) + a_2 \exp(-2\pi i x/\lambda) = a_1(-\xi)^{i\alpha} + a_2(-\xi)^{-i\alpha}, \ \alpha = l/\lambda. \tag{7}$$

As will be shown, the condition that the exact solution reduce approximately to these values for large values of x, suffices to determine it uniquely, and also to determine the constants a_1 and a_2. The quantity $\rho = |a_2/a_1|^2$ is the reflection coefficient, whose value is required for the applications mentioned in the first paragraph.

In working with the hypergeometric series, Eq. (5), it must be borne in mind that it converges only for $|y| < 1$. It then appears that of the twenty-four well-known ways[6] in which solutions of the hypergeometric equation can be expressed in terms of $F(a, b, c, y)$, only eight converge for large values of $\xi \, (x > 1)$; of these only four approach $(-\xi)^{i\beta}$ (the other four approaching $(-\xi)^{-i\beta}$) when $|\xi|$ increases indefinitely. The four solutions approaching $(-\xi)^{i\beta}$ are only formally different, so that it suffices to study any one of them; we single out the form

$$u = (1-\xi)^{i\beta}(\xi/\xi-1)^{i\alpha}F\left[\tfrac{1}{2} + i(\alpha-\beta+\delta),\right.$$
$$\left. -\tfrac{1}{2} + i(\alpha-\beta-\delta),\ 1-2i\beta,\ 1/(1-\xi)\right] \tag{8}$$

in which α and β have the values of Eqs. (6) and (7) and δ is to be defined immediately. If we define a quantity C by the relation $(2mC)^{1/2} = h/2l$, it becomes possible to write

$$\alpha = \tfrac{1}{2}(W/C)^{1/2}, \quad \beta = \tfrac{1}{2}[(W-A)/C]^{1/2}, \tag{9}$$

and the quantity δ is then defined by

$$\delta = \tfrac{1}{2}[(B-C)/C]^{1/2}. \tag{9a}$$

[6] Klein, pp. 76–80; Forsythe, pp. 189–194.

C is the energy of an electron whose de Broglie wave-length is $2l$, the total width of the region of variable potential.

The function u of Eq. (8) obviously approaches $(-\xi)^{i\beta}$ for large values of ξ, since $F(a, b, c, o) = 1$. Its value for very small values of ξ cannot be determined at once, however, since the series $F(a, b, c, 1)$ diverges. It is necessary to have recourse to the so-called process of analytic extension, and to express u in terms of series which do converge for small values of $|\xi|$. The result of the analytic extension of the hypergeometric series has been known, practically speaking, since the times of Euler and Gauss; it is summarized in the formula[7] for compounding two hypergeometric series:

$$\begin{aligned} y^a(1-y)^c F(a+b+c,\ a+b'+c,\ 1+a-a',\ y) \\ = \phi(c,c')(1-y)^c y^a F(a+b+c,\ a+b'+c,\ 1+c-c',\ 1-y) \\ + \phi(c',c)(1-y)^{c'} y^a F(a+b+c',\ a+b'+c',\ 1+c'-c,\ 1-y) \end{aligned} \quad (10)$$

where

$$\phi(c,c') = \frac{\Gamma(1+a-a')\Gamma(c'-c)}{\Gamma(1-a'-b-c)\Gamma(-a'-b'-c)} \cdot \quad (11)$$

This equation is an identity for those values of y for which all the series converge, and may be used as a definition of $F(a, b, c, y)$ for $|y|>1$, $|1-y|<1$. If we set y equal to $1/(1-\xi)$, $a=-a'=-i\beta$, $b=-b'=\frac{1}{2}+i\delta$, $c=-c'=i\alpha$, and

$$\begin{aligned} a_1 &= \frac{\Gamma(1-2i\beta)\Gamma(-2i\alpha)}{\Gamma[\frac{1}{2}+i(-\alpha-\beta-\delta)]\Gamma[\frac{1}{2}+i(-\alpha-\beta+\delta)]}, \\ a_2 &= \frac{\Gamma(1-2i\beta)\Gamma(+2i\alpha)}{\Gamma[\frac{1}{2}+i(\alpha-\beta-\delta)]\Gamma[\frac{1}{2}+i(\alpha-\beta+\delta)]}, \end{aligned} \quad (12)$$

it reduces to

$$\begin{aligned} u = a_1(\xi/\xi-1)^{i\alpha}(1-\xi)^{i\beta}F[\tfrac{1}{2}+i(\alpha-\beta+\delta), \\ -\tfrac{1}{2}+i(\alpha-\beta-\delta),\ 1+2i\alpha,\ \xi/(\xi-1)] \\ + a_2(\xi/\xi-1)^{-i\alpha}(1-\xi)^{i\beta}F[\tfrac{1}{2}+i(-\alpha-\beta+\delta), \\ -\tfrac{1}{2}+i(-\alpha-\beta-\delta),\ 1-2i\alpha,\ \xi/(\xi-1)]. \end{aligned} \quad (13)$$

The two series on the right side of this equation converge when $|\xi/(\xi-1)|<1$ hence certainly when $|\xi|<\frac{1}{2}$. For very small values of ξ the value of u may be computed from this equation, and is seen to be exactly the expression of Eq. (7) with a_1 and a_2 defined by Eqs. (12). Eqs. (8) and (13) thus define the function u for all real values of x; it may readily be shown that it satisfies[8] Eq. (4), and is finite, continuous, and possesses continuous derivatives

[7] Klein, pp. 88–91; Forsythe, pp. 194–201.

[8] For it is a linear function of two of Kummer's twenty-four solutions (cf. reference 6).

throughout this range. It is therefore the wave-function we are seeking, and the coefficient of reflection is hence

$$\rho = \left|\frac{a_2}{a_1}\right|^2 = \left|\frac{\Gamma[\frac{1}{2} + i(\delta - \beta - \alpha)]\Gamma[\frac{1}{2} + i(-\delta - \beta - \alpha)]}{\Gamma[\frac{1}{2} + i(\delta - \beta + \alpha)]\Gamma[\frac{1}{2} + i(-\delta - \beta + \alpha)]}\right|^2 \tag{14}$$

since $|\Gamma(2i\alpha)/\Gamma(-2i\alpha)|$ is obviously 1.

In the numerical evaluation of this formula the two cases, δ = real and δ = imaginary, are to be distinguished. These two cases are separated by the condition $B = C$; since B will in general be of the order of magnitude of W, the case of a real δ corresponds to a potential barrier whose region of inhomogeniety is wide compared to the wave-length of the incident electron (cf. Eq. (9)) while an imaginary δ corresponds to a narrow region of inhomogeniety.

If δ is real, the arguments of all the gamma-functions have the form $\frac{1}{2}+iv$, where v is real. It is known that[9]

$$|\Gamma(u + iv)| = \Gamma(u) \exp[-P(u,v)]$$

and that

$$\exp[P(\tfrac{1}{2}, v)] = [\cosh(\pi v)]^{1/2}.$$

Hence

$$\begin{aligned}\rho &= \frac{\cosh[\pi(\delta - \beta + \alpha)]\cosh[\pi(\delta + \beta - \alpha)]}{\cosh[\pi(\delta - \beta - \alpha)]\cosh[\pi(\delta + \beta + \alpha)]} \\ &= \frac{\cosh[2\pi(\alpha - \beta)] + \cosh[2\pi\delta]}{\cosh[2\pi(\alpha + \beta)] + \cosh[2\pi\delta]}.\end{aligned} \tag{15}$$

If δ is imaginary, both the numerator and denominator of Eq. (14) have the form

$$|\Gamma(u + iv)\Gamma(1 - u + iv)|$$

with $u = \frac{1}{2} + |\delta|$. Now,

$$\exp[P(u,v) + P(1 - u,v)] = [(\cosh 2\pi v - \cos 2\pi u)/2 \sin^2 \pi u]^{1/2}$$

and hence

$$\rho = \frac{\cosh[2\pi(\alpha - \beta)] + \cos[2\pi|\delta|]}{\cosh[2\pi(\alpha + \beta)] + \cos[2\pi|\delta|]}. \tag{15a}$$

The two Eqs. (15) and (15a) are identical, if it be remembered that

$$\cosh[2\pi\delta] = \cos[2\pi|\delta|]$$

[9] The formulae regarding $\Gamma(u+iv)$ which are used in the following are all to be found on pp. 23–25 of N. Nielsen, Handbuch der gammafunktion, (Leipzig, 1906).

when δ is imaginary; the separate derivation of the two is necessary, however, for $|\Gamma(u+iv)|$ is not an analytic function. The expressions for ρ are plotted in Fig. 2 for $B=8A$ and various values of l.

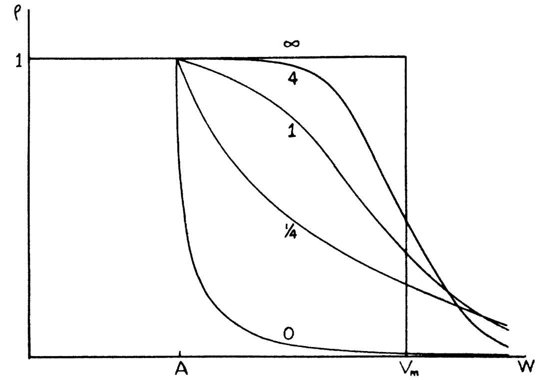

Fig. 2. Graphs of the reflection coefficient. The numbers are the values of A/C.

It is instructive to compare this expression for the reflection coefficient with the values which have been obtained by other writers. If $W<V_m$, the expression

$$1-\rho=\gamma\exp\left\{-\frac{4\pi}{h}\int(2m(V-W))^{1/2}dx\right\} \tag{16}$$

has been used, in which the integral is to be extended over all values of x for which $V>W$, and $\gamma\sim 1$. It may be shown that this is a valid approximation to Eq. (15) when l is very large, C very small. In this case, α and β become very large, so that

$$\cosh\left[2\pi(\alpha\pm\beta)\right]\sim\tfrac{1}{2}\exp\left[2\pi(\alpha\pm\beta)\right]$$

and $\delta\sim\frac{1}{2}(B/C)^{1/2}$. Hence, approximately,

$$\rho=\frac{1+\exp\left[\pi(W^{1/2}-(W-A)^{1/2}-B^{1/2})/C^{1/2}\right]}{1+\exp\left[\pi(W^{1/2}+(W-A)^{1/2}-B^{1/2})/C^{1/2}\right]}\,.$$

The argument of the exponential in the denominator of this expression is very much greater than 1 when $W\gg V_m$, and very much less than -1 when $W\ll V_m$. Hence

$$\rho=\exp\left[-\pi(W^{1/2}+(W-A)^{1/2}-B^{1/2})/C^{1/2}\right[\tag{17}$$

when $W\gg V_m$, and

$$(1-\rho)=\left\{1-\exp\left[-2\pi((W-A)/C)^{1/2}\right]\right\}$$
$$\exp\left[\pi(W^{1/2}+(W-A)^{1/2}-B^{1/2})/C^{1/2}\right]$$

when $W \ll V_m$. When l is very large, therefore, ρ is practically zero if $W > V_m$ and practically 1 if $W < V_m$; these formulae are valid except when $|W - V_m| \sim C$. Comparing the second of Eqs. (17) with Eq. (16) it is seen that the latter is verified if

$$-\frac{4\pi}{h}\int (2m(V - W))^{1/2}dx = \pi(W^{1/2} + (W - A)^{1/2} - B^{1/2})/C^{1/2}.$$

The integral on the left is readily evaluated by the method of residues,[10] and does prove to be equal to the right side of the equation.

For very small values of l (C very large) $\cosh 2\pi\delta$ approaches -1 regardless of B and

$$\cosh 2\pi(\alpha \pm \beta) = 1 + \pi^2[W^{1/2} \pm (W - A)^{1/2}]^2/8C$$

so that

$$\rho = [W^{1/2} - (W - A)^{1/2}]^2/[W^{1/2} + (W - A)^{1/2}]^2.$$

In this limit, therefore, all effect of the maximum of potential function vanishes and the reflection coefficient has the value characteristic of a rectangular potential barrier of infinite width,[11] and height A.

For values of W very much larger than A, B, or C,

$$\cosh [2\pi(\alpha - \beta)] \sim 1, \quad \cosh [2\pi(\alpha + \beta)] \sim \tfrac{1}{2} \exp [2\pi(W/C)^{1/2}],$$

so that

$$\rho = [1 + 2 \cosh (2\pi\delta)] \exp [-2\pi(W/C)^{1/2}].$$

For $W \leqq A$ the reflection coefficient is always unity, as may be most readily deduced from general principles.

[10] See, e.g., A. Sommerfeld, Atombau, (4th Ed. 1924), p. 772.

[11] See, e.g., W. Heisenberg, Physical Principles of the Quantum Theory (in course of publication.)