TRANSMISSION OF ELECTRONS THROUGH POTENTIAL BARRIERS

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ABSTRACT

It is shown that the application of the Wentzel-Kramers-Brillouin approximate solution of the wave equation to problems of the transmission of electrons through potential barriers leads to simple derivations of formulas for the transmission coefficient. This method may be applied systematically to potential barriers of arbitrary form.

1. NUMEROUS examples of the transmission of electrons through potential barriers may be found in the literature in connection with the theory of radioactive disintegration and emission of electrons from metals. In those cases in which the wave equation does not admit of elementary solutions the calculations become lengthy and laborious and it has been found necessary to introduce asymptotic properties of the solutions in order to arrive at results of physical interest. We have found that the same end results can be obtained by the use of the Wentzel-Kramers-Brillouin approximate solution of the wave equation. The calculations are much simplified and can be extended systematically to any problems of this type.

2. The W.K.B. solution possesses enough similarity to classical behaviour so that the physical interpretation of every step of the calculation is self-evident, yet it also possesses properties which are typically wave-mechanical.[2] If the one-dimensional wave equation be written in the form

$$\psi''(x) + (E - V(x))\psi(x) = 0 \tag{1}$$

the W.K.B. fundamental solutions may be written

$$\psi(x) = (E - V)^{-1/4} e^{\pm i\int (E-V)^{\frac{1}{2}} dx}. \tag{2}$$

This approximation is invalid in the neighborhood of values of x for which $E - V(x) = 0$, that is, where the classical kinetic energy vanishes. In regions where $E - V(x) > 0$ the solutions have an oscillatory character while in those regions where $E - V(x) < 0$ they behave as real exponentials. In order to have an approximate solution valid throughout the range of x we must know the correspondence between solutions of the oscillatory type in one region and those of the exponential type in an adjoining region. "Connection formulas" have been given by Kramers and Zwaan.[3] They require that

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[2] G. Wentzel, Zeits. f. Physik **38**, 518 (1926); L. Brillouin, C. R., Juli, 1926; H. A. Kramers, Zeits. f. Physik **33**, 828 (1926); L. A. Young and G. E. Uhlenbeck, Phys. Rev. **33**, 1154 (1930)

[3] H. A. Kramers, reference 2; A. Zwaan, Utrecht Dissertation, 1929.

$$\begin{aligned}(V-E)^{-1/4}e^{+\int(V-E)^{\frac{1}{2}}dx} &\longleftrightarrow (E-V)^{-1/4}\cos\left\{\int(E-V)^{1/2}dx-\frac{\pi}{4}\right\}\\ (V-E)^{-1/4}e^{-\int(V-E)^{\frac{1}{2}}dx} &\longleftrightarrow 2(E-V)^{-1/4}\cos\left\{\int(E-V)^{1/2}dx+\frac{\pi}{4}\right\}.\end{aligned} \tag{3}$$

The above integrals are to be taken between the limits x and x_1 $(E-V(x_1)=0)$ in such a way that the integrals are always positive. Since we are always interested in travelling waves we shall use an alternative form of the above.

$$\begin{aligned}(E-V)^{-1/4}e^{+i\int(E-V)^{1/2}dx} &\longleftrightarrow (V-E)^{-1/4}\left\{(i)^{1/2}e^{+\int(V-E)^{1/2}dx}+\tfrac{1}{2}(-i)^{1/2}e^{-\int(V-E)^{1/2}dx}\right\}\\ (E-V)^{-1/4}e^{-i\int(E-V)^{1/2}dx} &\longleftrightarrow (V-E)^{-1/4}\left\{(-i)^{1/2}e^{+\int(V-E)^{1/2}dx}+\tfrac{1}{2}(i)^{1/2}e^{-\int(V-E)^{1/2}dx}\right\}\end{aligned} \tag{4}$$

In the neighborhood of $x=x_1$ we may replace $E-V(x)$ by a linear function of x and use exact solutions which are expressible in terms of Bessel functions of order 1/3.

3. We shall first consider a case treated by Fowler and Nordheim,[4] that of an electron escaping from a metal into a uniform accelerating field (Fig. 1). We must consider the following cases: (a) $E>V_0$; (b) $E<V_0$; (c) $E=V_0$. Case (a).

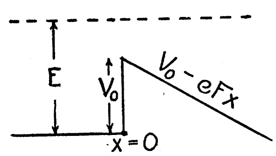

Fig. 1.

For $x<0$ we write for the incident electron beam

$$\psi_i = p^{-1/2}e^{ipx} \qquad p=\frac{2\pi}{\lambda}=\frac{2\pi}{h}(2mE)^{1/2} \tag{5}$$

for the reflected beam

$$\psi_r = bp^{-1/2}e^{-ipx}. \tag{6}$$

For $x>0$ we use the W.K.B. solution for an emerging wave

$$\psi_t = cy^{-1/4}e^{+i\int_0^x y^{\frac{1}{2}}dx} \tag{7}$$

where

$$y = p^2 - p_0^2 + \alpha x;\ p_0 = \frac{2\pi}{h}(2mV_0)^{1/2}$$

$$\alpha = \frac{8\pi^2 meF}{h^2}\cdot$$

The constants b and c are normalization factors and ψ_i is normalized for unit "current." At $x=0$ $><$ $\psi_i+\psi_r=\psi_t$ and $\psi_i'+\psi_r'=\psi_t'$

[4] R. H. Fowler and L. Nordheim, Proc. Roy. Soc. **A119**, 173 (1928).

$$
\begin{aligned}
1 + b &= cp^{1/2}y_0^{-1/4} \\
1 - b &= cp^{-1/2}\{y_0^{1/4} + i\alpha y_0^{-5/4}/4\} \qquad (8)\\
y_0 &= (y)_{x=0}.
\end{aligned}
$$

The transmission coefficient is defined as the ratio of transmitted to incident current i.e.

$$T = c\bar{c}$$

from Eqs. (8) we find immediately

$$T = \frac{4py_0^{1/2}}{[p + y_0^{1/2}]^2 + \left[\frac{\alpha}{4y_0}\right]^2} \qquad (9)$$

or in terms of energies

$$T = \frac{4(E(E - V_0))^{1/2}}{[E^{1/2} + (E - V_0)^{1/2}]^2 + \frac{e^2F^2}{16\kappa^2(E - V_0)^2}} \qquad \kappa^2 = \frac{8\pi^2 m}{h^2}. \qquad (10)$$

For an arbitrary $V(x)$ $(V(x) < V_0)$ the transmission coefficient may be obtained by replacing in (9) α by $(8\pi^2 m/h^2)(dV/dx)_{x=+0}$.

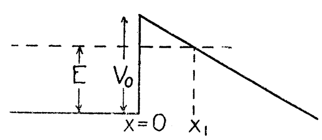

Fig. 2.

Case (b).

For this case it is convenient to normalize the transmitted "current" rather than the incident to unity. We have

$$
\left.
\begin{aligned}
\psi_i &= ap^{-1/2}e^{ipx} \\
\psi_r &= bp^{-1/2}e^{-ipx}
\end{aligned}
\right\} \quad x < 0 \qquad (11a)
$$

$$\psi_t = y^{-1/4}e^{i\int_{x_1}^{x} y^{1/2}dx} \quad x > x_1.$$

With the help of (4) we find for the region $0 < x < x_1$

$$
\begin{aligned}
\psi &= z^{-1/4}\{(i)^{1/2}e^{+\int_{x_1}^{x} z^{1/2}dx} + \tfrac{1}{2}(-i)^{1/2}e^{-\int_{x_1}^{x} z^{1/2}dx}\} \\
z &= -y.
\end{aligned} \qquad (11b)
$$

Boundary conditions at $x = 0$ yield

$$
\begin{aligned}
a + b &= p^{1/2}z_0^{-1/4}\{(i)^{1/2}A_+ + \tfrac{1}{2}(-i)^{1/2}A_-\} \\
a - b &= -ip^{-1/2}z_0^{-1/4}\left\{((i)^{1/2}A_+ - \tfrac{1}{2}(-i)^{1/2}A_-)z_0^{1/2} \right. \qquad (12)\\
&\qquad \left. + \frac{\alpha}{4z_0}\left((i)^{1/2}A_+ + \frac{(-i)^{1/2}}{2}A_-\right)\right\}
\end{aligned}
$$

where

$$A_+ = e^{+\int_{x_1}^{0} z^{1/2} dx}$$
$$A_- = e^{-\int_{x_1}^{0} z^{1/2} dx}. \tag{13}$$

Elimination of b from the above allows the evaluation of $a\bar{a}$. We find

$$a\bar{a} = \tfrac{1}{4} p z_0^{-1/2} A_+^2 \left\{ \left(1 + \frac{\alpha}{8pz_0} A_-^2 - \frac{1}{2p} z_0^{1/2} A_-^2 \right) + \left(\frac{z_0^{1/2}}{p} + \frac{\alpha}{4pz_0} - \frac{1}{2} A_-^2 \right) \right\}. \tag{14}$$

Examination of the relative orders of magnitudes of the bracketed terms shows that terms containing A_-^2 are negligible. The error introduced by dropping these terms increases as $E \rightarrow V_0$ but in this case the entire approximation becomes invalid since the critical point x_1 approaches $x=0$ where boundary conditions must be satisfied.

Due to our altered normalization the transmission coefficient for this case is

$$T = (a\bar{a})^{-1} = \frac{4pz_0^{1/2} A_-^2}{p^2 + \left(\dfrac{\alpha}{4z_0} + z_0^{1/2} \right)^2}. \tag{15}$$

We have

$$z = p_0^2 - p^2 - \alpha x$$
$$z_0 = p_0^2 - p^2$$
$$A_-^2 = e^{-4(p_0^2 - p^2)^{3/2}/3\alpha}.$$

We obtain, therefore

$$T = \frac{4(E(V_0 - E))^{1/2} e^{-4\kappa (V_0 - E)^{3/2}/3eF}}{E + \left(\dfrac{eF}{4\kappa (V_0 - E)} + (V_0 - E)^{1/2} \right)^2} \tag{16}$$

It is easy to see that for all values of the electric field F obtainable in practice the term in F can be neglected giving

$$T = \frac{4(E(V_0 - E))^{1/2}}{V_0} e^{-4\kappa (V_0 - E)^{3/2}/3eF} \tag{17}$$

in agreement with the final results of Fowler and Nordheim.[4] Eq. (15) may be generalized for an arbitrary $V(x)$ ($V(x) < V_0$) just as in the case of Eq. (9).
Case (c).

This case cannot be treated by the W.K.B. approximate method but it is easy to treat it exactly in the following manner. For $x<0$ we write as usual

$$\psi_i = p^{-1/2} e^{ipx} \quad \psi_r = b p^{-1/2} e^{-ipx}. \tag{18}$$

For $x>0$ we have the wave equation

$$\psi_t'' + \alpha x \psi_t = 0. \tag{19}$$

The solution of this equation for small values of x which represents an outgoing beam for large x may be written:

$$\psi_t = c(1 - \beta e^{-i\pi/3}x) \tag{20}$$

where

$$\beta = \frac{\Gamma\left(\frac{2}{3}\right)}{\Gamma\left(\frac{4}{3}\right)} \left(\frac{\alpha}{9}\right)^{1/3} = \frac{\Gamma\left(\frac{2}{3}\right)}{\Gamma\left(\frac{4}{3}\right)} \left(\frac{\kappa^2 eF}{9}\right)^{1/3}. \tag{21}$$

The boundary conditions at $x=0$ yield

$$\begin{aligned} 1 + b &= cp^{1/2} \\ 1 - b &= -ic\beta p^{-1/2}e^{-i\pi/3}. \end{aligned} \tag{22}$$

The transmission coefficient

$$T = 1 - b\bar{b} = \frac{4p\beta \sin\frac{\pi}{3}}{p^2 + \beta^2 + 2p\beta \sin\frac{\pi}{3}} \tag{23}$$

It is easy to show that the above expression is still valid for more general potentials if F is taken as the field at $x=0$.

4. As our next example we will consider a potential barrier with external retarding field of the type indicated in Fig. 3.

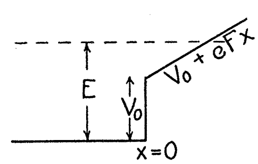

Fig. 3.

It is clear that in this case there will be no transmitted current and that only electrons possessing energies greater than V_0 will contribute appreciably to the charge density for $x>0$. Only these electrons will be considered. As usual we write for the incident and reflected beams ($x<0$).

$$\psi_i = p^{-1/2}e^{ipx} \quad \psi_r = bp^{-1/2}e^{-ipx}.$$

For $x>x_1$ where $x_1=(E-V_0)/eF$ we write for the transmitted electrons (no current!)

$$\psi_t = \frac{de^{-\int_{x_1}^{x} z^{1/2}dx}}{2z^{1/4}} \tag{24}$$

$$z = -y$$

$$y = p^2 - p_0^2 - \alpha x.$$

Making use of the connection Eqs. (3) we find for the region $0<x<x_1$.

$$\psi = dy^{-1/4} \cos \left\{ \int_x^{x_1} y^{1/2} dx + \frac{\pi}{4} \right\}. \tag{25}$$

This represents a stationary wave in this region. Boundary conditions at $x=0$ give

$$\begin{aligned} 1 + b &= dp^{1/2} y_0^{-1/4} \cos A \\ 1 - b &= -idp^{-1/2} y_0^{-1/4} \left\{ \frac{\alpha}{4y_0} \cos A + y_0^{1/2} \sin A \right\} \end{aligned} \tag{26}$$

where

$$A = \int_0^{x_1} y^{1/2} dx + \frac{\pi}{4} = \frac{2}{3\alpha} y_0^{3/2} + \frac{\pi}{4}$$

we find

$$d\bar{d} = \frac{4y_0^{1/2}}{p \left\{ \cos^2 A + \dfrac{1}{p^2} \left(\dfrac{\alpha \cos A}{4y_0} + \sin A \right)^2 \right\}}. \tag{27}$$

Since A varies extremely rapidly with p we may take the average values of the trigonometric terms in the denominator to obtain

$$\overline{(d\bar{d})}_{(\Delta p)} = \frac{8y_0^{1/2}}{p \left\{ 1 + \dfrac{1}{p^2} \left(\dfrac{\alpha^2}{16y_0^2} + 1 \right) \right\}}. \tag{28}$$

The average charge density over the range Δp is

$$\overline{\psi\bar{\psi}}_{(\Delta p)} = \overline{(d\bar{d})}_{\Delta p} y^{-1/2} \cos^2 \left\{ \int_x^{x_1} y^{1/2} dx + \frac{\pi}{4} \right\}. \tag{29}$$

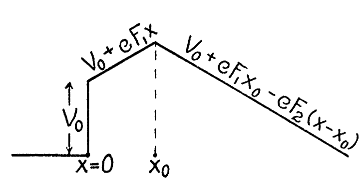

Fig. 4.

Since the space periodicity is approximately λ, the de Broglie wave-length, we may replace $\cos^2\{\int_x^{x_1} y^{1/2}dx+\pi/4\}$ by 1/2 to obtain

$$\overline{\psi\bar{\psi}}_{(\Delta p, \Delta x)} = \frac{4(y_0/y)^{1/2}}{p \left\{ 1 + \dfrac{1}{p^2} \left(\dfrac{\alpha^2}{16y_0^2} + 1 \right) \right\}}. \tag{30}$$

The above results allow a complete discussion of the following case (Fig. 4).

This form of potential curve approximates the space charge condition in vacuum tubes. The retarding field acts effectively to increase the work function.

5. In conclusion we shall consider two cases where the form of potential barrier is modified by an image field. The first example is illustrated by Fig. 5. For $x<x_0$ $V(x)=0$ and for $x>x_0$ $V(x)=V_0-e^2/4x$. Nordheim[5] determines x_0 by $V_0=e^2/4x_0$. We can find the transmission by using the generalization of Eq. (9).

$$T=\frac{4py_0^{1/2}}{[p+y_0^{1/2}]^2+\left[\dfrac{\alpha}{4y_0}\right]^2}=\frac{4E}{4E+\left(\dfrac{V_0^2}{\kappa e^2E}\right)^2}=\frac{1}{1+\dfrac{V_0^4}{16RhE^3}} \tag{31}$$

It is interesting to note that Rh, the ionization energy of hydrogen, enters naturally because of the occurrence of a hydrogenic potential in the wave equation. This formula is valid for $E\geqq V_0$ since $y>0$ throughout the finite region of x. Anyone who has attempted to follow Nordheim's calculations will

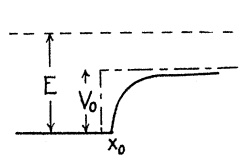

Fig. 5.

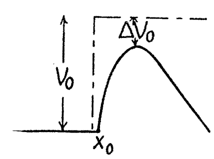

Fig. 6.

see immediately the advantages of the method used here. As our last example we will consider the example of image field plus a uniform accelerating field (Fig. 6). For $x<x_0$ $V(x)=0$ for $x>x_0$

$$V(x)=V_0-\frac{e^2}{4x}-eFx$$

$$\Delta V_0=+(e^3F)^{1/2}.$$

The generalization of (9) for all electrons possessing energies greater than $V-\Delta V_0$ gives

$$T=\frac{4E^{1/2}\left(E+\dfrac{e^3F}{4V_0}\right)^{1/2}}{\left\{E^{1/2}+\left(E+\dfrac{e^3F}{4V_0}\right)^{1/2}\right\}^2+\left\{\dfrac{e^3F-4V_0^2}{4\kappa\left(E+\dfrac{e^3E}{4V_0}\right)}\right\}^2}. \tag{32}$$

It is hoped that these examples will indicate the advantages of the use of the W.K.B. approximation in problems of this type and will suffice to facilitate its application to other cases of interest.

[5] L. Nordheim, Proc. Roy. Soc. **A121**, 626 (1928).