a relatively simple derivation of the Bloch equation, there does not seem to be much point in trying to improve this theory, if at the same time it becomes more complicated.

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Quantum-Mechanical Tunneling

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An elementary method is given for the exact determination of the quantum mechanical transmission and reflection coefficients for a rectangular one-dimensional potential barrier. The method also finds application in approximate solutions for multistep barriers.

THE method commonly used in calculating the transmission and reflection coefficients for a particle incident at a rectangular one-dimensional potential barrier, (see, e.g., Condon[1]) depends on solving the Schrödinger equation for the region within the barrier and on either side, and eliminating the two constants which were introduced in the solution for the region within the barrier. Solutions for barriers with several steps involve the elimination of two constants for each region of constant potential within the barrier. In all cases, the constants are eliminated by using the conditions for continuity of ψ and $d\psi/dx$ at the discontinuities in potential. The treatment to be found in modern books on the subject (e.g., Merzbacher,[2] and Dicke and Wittke[3]) is usually that for a symmetrical barrier and in some cases is only approximate.

The present method consists, firstly, in writing down the reflected and the transmitted components of an elementary wavefunction ψ incident at each discontinuity of potential to be found in the barrier. The resultant ψ wave in a region of interest is then calculated, following the principle of superposition, by summing in a geometric series the components resulting from multiple reflection and transmission. In this way, one arrives easily at the transmission and reflection coefficients for the barrier without the introduction of unnecessary constants and the necessity for their subsequent elimination. An approximate solution for the case of a multistep barrier is found by including only those terms of the series which are found to be of appreciable size.

The solution of the Schrödinger equation $H\psi = E\psi$ for a particle in a region of constant potential energy V may be written as

$$\psi = \exp(ikx), \quad (1)$$

where

$$k = [2m(E-V)]^{\frac{1}{2}}/h. \quad (2)$$

For $E > V$, k is real and the solution represents a complex harmonic wave traveling in the direction of increasing x; while if $E < V$, the physically meaningful solution for ψ is an exponentially decreasing real function of x. (For $E = V$, $\psi = 1$, representing a stationary particle of undetermined position.) Thus, for the present purpose,

[1] E. U. Condon, Rev. Mod. Phys. **3**, 43–74 (1931).
[2] E. Merzbacher, *Quantum Mechanics* (John Wiley & Sons, Inc., New York, 1961), pp. 91–92.
[3] R. H. Dicke and J. P. Wittke, *Introduction to Quantum Mechanics* (Addison-Wesley Publ. Co., Inc., Reading, Mass., 1960), pp. 40–46.

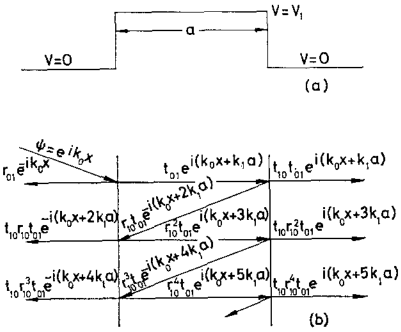

FIG. 1. (a) Symmetrical rectangular potential barrier and (b) wavefunctions resulting from the incident ψ by successive transmission and reflection.

we may adopt $\psi=\exp(ikx)$ as a general form of solution, where k may be real or imaginary.

Let a particle which is incident from the left at a discontinuity in potential at $x=0$ be represented by the wavefunction $\psi=\exp(ik_1x)$, where the momentum of the particle $p_1=\hbar k_1$, and the transmitted and the reflected components by $t_{12}\exp(ik_2x)$ and $r_{12}\exp(-ik_1x)$, respectively. Continuity of ψ and $d\psi/dx$ at $x=0$ gives

$$t_{12}=2k_1/(k_1+k_2) \quad r_{12}=(k_1-k_2)/(k_1+k_2), \tag{3}$$

where

$$k_1=[2m(E-V_1)]^{\frac{1}{2}}/\hbar$$

and

$$k_2=[2m(E-V_2)]^{\frac{1}{2}}/\hbar. \tag{4}$$

In the case of the symmetrical barrier shown in Fig. 1 (a), the amplitude coefficients for the first and second discontinuities are seen to be

$$\begin{aligned} t_{01}=2k_0/(k_0+k_1) \quad & t_{10}=2k_1/(k_1+k_0), \\ r_{01}=&(k_0-k_1)/(k_0+k_1), \\ r_{10}=&(k_1-k_0)/(k_1+k_0), \end{aligned} \tag{5}$$

and the multiply reflected and transmitted terms are those shown in Fig. 1 (b). The transmitted or the reflected wavefunction is calculated by summing the relevant terms. Taking the transmitted wavefunctions, one obtains

$$\begin{aligned} \psi_{\text{trans}}=&t_{10}t_{01}\exp[i(k_0x+k_1a)] \\ &+t_{10}r_{10}^2t_{01}\exp[i(k_0x+3k_1a)] \\ &+t_{10}r_{10}^4t_{01}\exp[i(k_0x+5k_1a)]+\cdots \end{aligned} \tag{6}$$

$$\begin{aligned} =t_{10}t_{01}\exp[i(k_0x+k_1a)]\{1+r_{10}^2\exp(2ik_1a) \\ +r_{10}^4\exp(4ik_1a)+\cdots\}, \end{aligned} \tag{7}$$

i.e.,

$$\psi_{\text{trans}}/\psi_{\text{inc}} =t_{10}t_{01}\exp(ik_1a)/[1-r_{10}^2\exp(2ik_1a)], \tag{8}$$

which, on substituting for t_{01}, t_{10}, and r_{10} from Eq. (5), gives

$$\psi_{\text{trans}}/\psi_{\text{inc}}=4k_0k_1\exp(ik_1a)/ [(k_0+k_1)^2-(k_1-k_0)^2\exp(2ik_1a)]. \tag{9}$$

Hence, the intensity transmission coefficient for the barrier

$$\begin{aligned} T=&|\psi_{\text{trans}}/\psi_{\text{inc}}|^2 \\ =&|4k_0k_1/[(k_0+k_1)^2\exp(-ik_1a) \\ &-(k_1-k_0)^2\exp(ik_1a)]|^2, \end{aligned} \tag{10}$$

where k_0 is real and k_1 may be real or pure imaginary, as given by Eq. (4).

This approach is readily extended for the case of the double barrier shown in Fig. 2 (a). Analysis of the first barrier enables us to write $\psi=t\exp(ik_0x)$ for the transmitted wavefunction, where t, which includes a phase shift term, is given by Eq. (9). The action of the second barrier on this wavefunction is to give rise to the succession of terms shown in Fig. 2 (b), where r is the amplitude reflection coefficient for the complete single barrier. The wavefunction transmitted by the complete barrier system is found by summing as before. The conditions which give rise to resonance effects in the system may be readily seen from phase considerations.

The case of the asymmetrical barrier which is specified by the three regions of potential V_1, V_2, and V_3, as shown in Fig. 3, is treated in the

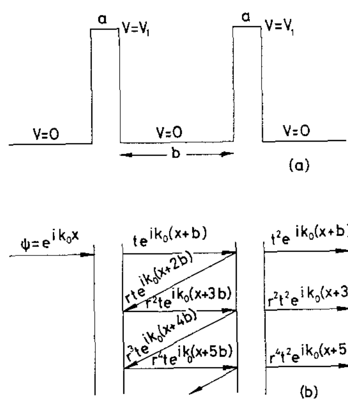

FIG. 2. (a) Symmetrical double potential barrier and (b) the components giving rise to a transmitted wave function.

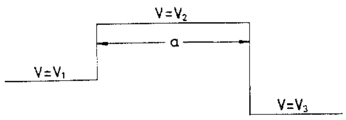

FIG. 3. Asymmetrical rectangular potential barrier.

same manner as the symmetrical barrier above, the summations giving rise to geometrical series as before. The relevant coefficients are

$$t_{pq}=2k_p/(k_p+k_q)\quad r_{pq}=(k_p-k_q)/(k_p+k_q), \tag{11}$$

where the suffixes refer to the three regions of the barrier. Writing the wavefunction incident from the left as $\psi=\exp(ik_1x)$ and summing this time over the reflected components, it is easily seen that

$$\psi_{\text{refl}}=r_{12}\exp(-ik_1x)+t_{21}r_{23}t_{12}\times\exp[-i(k_1x+2k_2a)]+t_{21}r_{23}r_{21}r_{23}t_{12}\times\exp[-i(k_1x+4k_2a)]+\cdots, \tag{12}$$

where

$$k_p=[2m(E-V_p)]^{\frac{1}{2}}/h, \tag{13}$$

i.e.,

$$\psi_{\text{refl}}=\exp(-ik_1x)\{r_{12}+t_{21}r_{23}t_{12}\exp(-i2k_2a)\times[1+r_{21}r_{23}\exp(-i2k_2a)+r_{21}^2r_{23}^2\times\exp(-i4k_2a)+\cdots]\}; \tag{14}$$

or, on substituting from Eq. (11) and summing, $\psi_{\text{refl}}/\psi_{\text{inc}}$

$$=[k_1-k_2+4k_1k_2(k_2-k_3)/(k_1+k_2)(k_2+k_3)\times\exp(i2k_1a)-(k_2-k_1)(k_2-k_3)]\times(k_1+k_2)^{-1}. \tag{15}$$

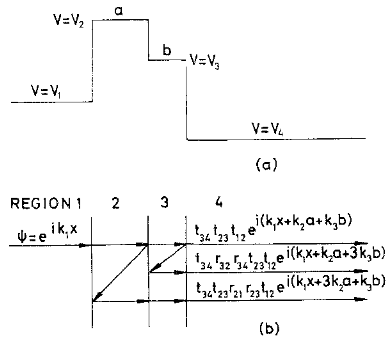

FIG. 4. (a) Multistep potential barrier and (b) the formation of the three dominant terms of the transmitted wavefunction.

Approximate solutions may be arrived at in cases of more complex barriers by summing the terms of significant size for the various modes of transmission as is, e.g., indicated in Fig. 4, where the first three terms of the transmitted wavefunction are shown. Owing to the multiplicity of path type, this approach is of course practicable only when the size of the terms falls rather sharply. Approximate solutions may similarly be found for the cases where a smoothly varying potential function allows a reasonably good stepwise approximation to be made.

In conclusion, it may be said that the method offers a simple alternative solution to barrier penetration problems, and because of its analogy with the analysis of reflection and transmission by thin films in physical optics, is likely to prove attractive to students.