Note on the Transmission and Reflection of Wave Packets by Potential Barriers

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In previous studies, by the methods of wave mechanics, of one-dimensional motion of particles in cases in which there are intervals in which the value of the potential energy function $V(x)$ exceeds the value of the total energy E, attention has been confined to wave functions of the form $f(x, E) \exp(-2\pi iEt/h)$. In the present note wave packets are considered, instead of these trains of waves.

The function $V(x)$ is taken as follows:

$$V(x) = 0 \text{ for } x < 0 \text{ and for } x > a,$$
$$= V_0 > 0 \text{ for } 0 < x < a.$$

A wave function is set up which initially represents a wave packet moving toward the point $x=0$ from the left. The separation of the incident packet into a reflected packet and a transmitted packet is studied. It is found that the transmitted packet appears at the point $x=a$ at about the time at which the incident packet reaches the point $x=0$, so that there is no appreciable delay in the transmission of the packet through the barrier.

The recent literature on wave mechanics contains a large number of papers dealing with the one-dimensional motion of particles in cases in which the potential energy function, $V(x)$, has various arrangements of large and small values. According to classical mechanics, if the value of $V(x)$ at each point of a certain interval exceeds the value of the total energy, E, of the particle, the particle can neither enter nor pass through that interval. It is for this reason that such an interval, or the function $V(x)$ in such an interval, is called a "potential barrier." According to quantum mechanics a potential barrier is not an absolute barrier to particles with small total energy; such a particle may either be reflected or transmitted by the barrier.

Apparently, in all of the work which has been done hitherto on problems concerning potential barriers, attention has been confined to solutions of the wave equation which are of the form

$$\Psi = f(x, E) \exp(-2\pi iEt/h).$$

As is known, such solutions apply to cases in which the particle has the precisely determined value E of total energy and in which the relative probabilities of finding the particle in various intervals are independent of the time. The typical problem which has been considered heretofore may be stated as follows: Assuming that the particle is moving toward a certain potential barrier with total energy E, what is the probability that it will pass through the barrier?

The solution of such a problem can give no information about the manner in which the particle traverses the barrier, when it does. It has been pointed out by Condon[1] that it would be interesting to consider problems, involving

[1] Condon, Revs. Mod. Phys. 3, 76 (1931).

potential barriers, in which the relative probabilities of finding the particle in various intervals are not independent of the time. It is only in the sense of studying such probabilities that we can investigate, by the methods of wave mechanics, the transmission of a particle through a barrier. The present note is devoted to the study of a simple typical problem of the kind suggested by Condon.

We shall employ the potential energy function which is defined by the equations

$$\left.\begin{aligned} V(x) &= 0 && x < 0, \\ &= V_0 > 0 && 0 < x < a, \\ &= 0 && x > a. \end{aligned}\right\} \tag{1}$$

We shall take a suitable elementary wave function of the form $f(x, E)$ $\exp\left[-2\pi iEt/h\right]$ and effectively integrate it with respect to E over a certain range, thus producing a new wave function. It is required that at $t=0$ this wave function shall form a wave packet, the bulk of which lies to the left of the point $x=0$ and is moving toward the barrier. The problem is to study the way the wave function changes with time, and, in particular, to study the development of the function in the interval $x>a$. There arises the question of whether we should select the elementary wave function and the interval of integration so that the resulting wave function shall initially be identically zero in the interval $x>a$, or so that no values of E greater than V_0 shall occur in the composition of the function, that is, so that the function $V(x)$ shall be definitely a barrier. The second of these choices is the one made here, because it seems on the whole to represent the more interesting situation, and because it leads to the simpler analysis. Of course, this choice gives us initially a certain non-zero value of the probability that the particle be in the interval $x>a$. But, as this value is small compared with the initial value of the probability that the particle be in the interval $x<0$, and compared with the final value of the probability that the particle be in the interval $x>a$, no real difficulty is created by the fact that this initial value is not zero.

As the exact solution of the problem is expressed in terms of definite integrals which are difficult to evaluate numerically, the discussion is confined to the simpler qualitative features of the wave function. This discussion suffices to give a rather clear idea of the properties of the solution.

The chief result of the study can be stated as follows: The probability that the particle be in the interval $x>a$ is initially small; as time goes on this probability increases, rather slowly at first, much more rapidly in the neighborhood of the time at which the bulk of the incident wave packet reaches the point $x=0$, and then more slowly again; the time interval during which this probability undergoes its chief variation is substantially independent, both as to location and as to length, of the height and width of the barrier.

Consider the function $\Psi(x, t)$ which is defined by the following sequence of equations:

$$\left.\begin{aligned}\Psi &= \Psi_1 + \Psi_2, & x &< 0,\\ &= \Psi_3 + \Psi_4, & 0 &< x < a,\\ &= \Psi_5, & x &> a;\end{aligned}\right\} \tag{2}$$

$$\left.\begin{aligned}
\Psi_1 &= \int_{w_1}^{w_2} \exp\left[-(w - E_0^{1/2})^2/(4\lambda^2) + ik(x + x_0)w - 2\pi i t w^2/h\right]dw,\\
\Psi_2 &= \int_{w_1}^{w_2} \beta_1(w^2)\exp\left[-(w - E_0^{1/2})^2/(4\lambda^2) - ik(x - x_0)w - 2\pi i t w^2/h\right]dw,\\
\Psi_3 &= \int_{w_1}^{w_2} \alpha_2(w^2)\exp\left[-(w - E_0^{1/2})^2/(4\lambda^2) + kx(V_0 - w^2)^{1/2}\right.\\
&\qquad \left. + ikx_0 w - 2\pi i t w^2/h\right]dw,\\
\Psi_4 &= \int_{w_1}^{w_2} \beta_2(w^2)\exp\left[-(w - E_0^{1/2})^2/(4\lambda^2) - kx(V_0 - w^2)^{1/2}\right.\\
&\qquad \left. + ikx_0 w - 2\pi i t w^2/h\right]dw,\\
\Psi_5 &= \int_{w_1}^{w_2} \alpha_3(w^2)\exp\left[-(w - E_0^{1/2})^2/(4\lambda^2) + ik(x + x_0 - a)w - 2\pi i t w^2/h\right]dw;
\end{aligned}\right\} \tag{3}$$

$$\left.\begin{aligned}
\beta_1(w^2) &= -1 - 2i\sin\theta\,\frac{ch[ka(V_0 - w^2)^{1/2} - i\theta]}{sh[ka(V_0 - w^2)^{1/2} - 2i\theta]},\\
\alpha_2(w^2) &= -i\sin\theta\,\frac{\exp[-ka(V_0 - w^2)^{1/2} + i\theta]}{sh[ka(V_0 - w^2)^{1/2} - 2i\theta]},\\
\beta_2(w^2) &= -i\sin\theta\,\frac{\exp[ka(V_0 - w^2)^{1/2} - i\theta]}{sh[ka(V_0 - w^2)^{1/2} - 2i\theta]},\\
\alpha_3(w^2) &= \frac{-i\sin 2\theta}{sh[ka(V_0 - w^2)^{1/2} - 2i\theta]},\\
\theta &= \arctan\left[w/(V_0 - w^2)^{1/2}\right].
\end{aligned}\right\} \tag{4}$$

Here λ, x_0, w_1, E_0, and w_2, are positive numbers, and

$$0 < w_1 < E_0^{1/2} < w_2 < V_0^{1/2}.$$

We write

$$8\pi^2 m/h^2 = k^2,$$

where m is the mass of the particle under consideration.

It is easy to verify that the function $\Psi(x, t)$ satisfies the Schrödinger non-relativistic wave equation

$$\frac{\partial^2\Psi}{\partial x^2} - k^2\left[V(x) + \frac{h}{2\pi i}\frac{\partial}{\partial t}\right]\Psi = 0,$$

and that, for any fixed value of t, Ψ and $\partial\Psi/\partial x$ are continuous functions of x.[2]

[2] Of course, the solution is set up by the familiar device of obtaining an elementary solution of the form $f(x, w)\exp(-2\pi i t w^2/h)$, and then integrating with rsepect to w. The limits of integration are taken as w_1, w_2, rather than 0, $V_0^{1/2}$, merely in order to make the problem of verifying the solution a little simpler.

The integrals in Eqs. (3) are difficult to evaluate numerically; we shall merely discuss them qualitatively, avoiding certain extreme values of the parameters a, V_0, E_0, λ, w_1, w_2. To state the complicated facts rather loosely, it will be shown that when $t=0$ the function Ψ is a packet of waves concentrated about the point $x=-x_0$. As t increases the packet moves to the right, gradually spreading out. The bulk of the packet strikes the barrier, that is, reaches the point $x=0$, at about the time $t=x_0[2E_0/m]^{-1/2}$ and the packet then separates into a reflected packet and a transmitted packet. The reflected packet moves indefinitely to the left. The transmitted packet starts to the right from the point $x=a$ when the original packet strikes the barrier. The transmitted packet, as it leaves the point $x=a$, is of substantially the same form, except for a constant factor, as the original packet when it reaches the point $x=0$. In the interval $0<x<a$ the function Ψ is nearly a monotonic decreasing function of x multiplied by a function of t which is small when $t=0$, has appreciable values in the neighborhood of the instant $t=x_0[2E_0/m]^{-1/2}$, and ultimately becomes small again.

To a great extent, the qualitative properties of Ψ can be deduced from those of the function Ψ_1. Hence, we shall first consider the latter function.

If $E_0^{1/2}-w_1$ and $w_2-E_0^{1/2}$ are fairly large, and if λ is not too large, we can write approximately

$$\Psi_1 = \int_{-\infty}^{\infty} \exp\left[-(w-E_0^{1/2})^2/(4\lambda^2)+ik(x+x_0)w-2\pi i t w^2/h\right]dw. \quad (5)$$

In order that this approximation shall be legitimate we must assume that the numbers

$$(E_0^{1/2}-w_1)/(2\lambda),\quad (w_2-E_0^{1/2})/(2\lambda),$$

are sufficiently large, say somewhat greater than unity. We make this assumption.

From (5) one obtains the following relation by means of some elementary transformations.

$$\begin{aligned}\exp\left[E_0/(4\lambda^2)-[E_0^{1/2}+2i\lambda^2k(x+x_0)]^2/[4\lambda^2(1+8\pi i\lambda^2t/h)]\right]\Psi_1 \\ = 2\lambda[-(1+8\pi i\lambda^2t/h)]^{-1/2}\int_{-\infty[-(1+8\pi i\lambda^2t/h)]^{1/2}}^{\infty[-(1+8\pi i\lambda^2t/h)]^{1/2}} \exp w^2dw.\end{aligned}$$

The limits of integration indicate that the path of integration is the entire straight line passing through the points $w=\pm[-(1+8\pi i\lambda^2t/h)]^{1/2}$. It can be shown without difficulty that the value of the integral in the right-hand member of the preceding equation is $i\pi^{1/2}$. Hence, we have the following approximate expression for the function defined by the first of Eqs. (3):

$$\begin{aligned}\Psi_1 = 2\lambda\pi^{1/2}(1+8\pi i\lambda^2t/h)^{-1/2}\exp\big[&-E_0/(4\lambda^2) \\ &+[E_0^{1/2}+2i\lambda^2k(x+x_0)]^2/[4\lambda^2(1+8\pi i\lambda^2t/h)]\big]. \quad (6)\end{aligned}$$

The principal qualitative properties of the function Ψ_1 can be obtained readily from the approximation (6). Let us consider the absolute magnitude of Ψ_1. We have, approximately, by (6),

$$|\Psi_1| = 2\lambda\pi^{1/2}(1 + 64\pi^2\lambda^4t^2/h^2)^{-1/4} \exp\,[(1 + 64\pi^2\lambda^4t^2/h^2)^{-1} \cdot [E_0 - 4\lambda^4k^2(x + x_0)^2 + 32\pi\lambda^4k(x + x_0)E_0^{1/2}t/h](4\lambda^2)^{-1} - E_0/(4\lambda^2)].$$

This shows that, for any fixed value of t, $|\Psi_1|$ has its greatest value near the point determined by the equation

$$x + x_0 = 4\pi k^{-1}E_0^{1/2}t/h = (2E_0/m)^{1/2}t.$$

At the point where $|\Psi_1|$ is a maximum we have approximately

$$|\Psi_1| = 2\lambda\pi^{1/2}(1 + 64\pi^2\lambda^4t^2/h^2)^{-1/4}.$$

It is to be observed that we have approximately

$$\Psi_1(x, 0) = 2\lambda\pi^{1/2} \exp\,[-\lambda^2k^2(x + x_0)^2 + ik(x + x_0)E_0^{1/2}].$$

The chief qualitative properties of the function Ψ_1 are now apparent. When $t=0$ the function is a packet of complex waves which is extremely small except in the neighborhood of the point $x=-x_0$. As t increases the packet moves to the right with speed which can be estimated as equal to $(2E_0/m)^{1/2}$. As the packet moves forward it spreads out, and the maximum absolute value of the function Ψ_1 diminishes.

If, as we assume, E_0 and V_0-E_0 are large, and a is not too large, the functions $\beta_1(w^2)$ and $\alpha_3(w^2)$ vary only slowly in the neighborhood of the point $w=E_0^{1/2}$, which is the important part of the interval of integration $w_1 \leqq w \leqq w_2$. Hence, we can write, approximately,

$$\Psi_2(x, t) = \beta_1(E_0)\Psi_1(-x, t), \tag{7}$$

$$\Psi_5(x, t) = \alpha_3(E_0)\Psi_1(x - a, t). \tag{8}$$

According to (7), the function Ψ_2 is approximately, aside from a constant factor, merely the function Ψ_1 with the sign of x changed. We now perceive the qualitative nature of the function Ψ in the interval $x<0$. Initially we have a packet of waves concentrated about the point $x=-x_0$. As t increases the packet travels to the right, gradually spreading out and diminishing in maximum absolute magnitude. The bulk of the packet reaches the barrier at $x=0$ at about the instant $t=(2E_0/m)^{-1/2}x_0$. Thereafter, the packet is multiplied by a nearly constant factor, and it travels indefinitely to the left, gradually spreading out as before.

Eq. (8) displays the nature of the function Ψ in the interval $x>a$. Initially the function is small throughout the interval. In the neighborhood of the instant $t=(2E_0/m)^{-1/2}x_0$ the function begins to have appreciable values in the neighborhood of the point $x=a$. Thereafter we have a wave packet moving off indefinitely to the right, and gradually flattening out. As the function $\alpha_3(w^2)$ is small throughout the more important part of the interval of integration, the packet which moves to the right from the barrier is smaller than the packet which impinges on the barrier from the left.

It is significant that $\Psi(x, t)$ first attains appreciable values in the interval $x>a$ when the bulk of the incident packet reaches the point $x=0$. In this connection it is interesting to compute the probability $P(t)$ that the particle be in the interval $x>a$ at the instant t. It is easily found, on the basis of the approximations already made, that

$$P(t) = \int_a^\infty |\Psi_5(x, t)|^2 dx = 2^{3/2}\pi\lambda k^{-1} |\alpha_3(E_0)|^2 \int_\Omega^\infty e^{-u^2} du, \tag{9}$$

where

$$\Omega = 2^{1/2}\lambda[hkx_0 - 4\pi E_0^{1/2}t][h^2 + 64\pi^2\lambda^4 t^2]^{-1/2}. \tag{10}$$

These equations show that, to within the accuracy of the qualitative discussion given, the probability $P(t)$ does not depend on the height or width of the barrier, except through the constant factor $|\alpha_3(E_0)|^2$. In particular, the instant of most rapid increase of $P(t)$ is independent of V_0 and a.

It remains to examine $\Psi(x, t)$ in the interval $0<x<a$.

On the assumption that $ka(V_0-E_0)^{1/2}$ is fairly large, the function $\beta_2(w^2)$ is much larger, numerically, than $\alpha_2(w^2)$ throughout the more important part of the interval of integration. It follows that Ψ_4 is larger than Ψ_3 in the interval $0<x<a$, except, possibly near the point $x=a$ where both functions are small. Hence, throughout most of the interval $0<x<a$ the function Ψ is nearly equal to Ψ_4.

Now, throughout the more important part of the interval of integration $\exp[-kx(V_0-w^2)^{1/2}]$ is a slowly varying function of w. Therefore, we can write approximately,

$$\Psi_4 = \exp[-kx(V_0 - E_0)^{1/2}] \int_{w_1}^{w_2} \beta_2(w^2) \exp[-(w - E_0^{1/2})^2/(4\lambda^2) + ikx_0 w - 2\pi i t w^2/h] dw. \tag{11}$$

This equation shows that $|\Psi_4|$ is approximately a monotonic function of x multiplied by a function of t. The fact that Ψ is a continuous function of x, together with the facts which we have already deduced concerning Ψ in the intervals $x<0$ and $x>a$, shows that the function of t must be small when $t=0$, must attain appreciable values in the neighborhood of the instant $t=(2E_0/m)^{-1/2}x_0$, and must ultimately become small again.

In conclusion a word should be said about two physically important limiting cases which immediately come to mind. These are the cases in which we have $V_0=0$ and $V_0=\infty$, respectively.

The present theory is in no way applicable to the case $V_0=0$. In order to treat this case we would have to consider cases in which the wave packet contains elementary wave functions pertaining to values of E which are greater than V_0. However, for the sake of simplicity, and in order to confine the discussion to those problems that seem to possess the most interesting features, such cases have been explicitly excluded from consideration in this paper.

On the other hand, the theory does apply to the case in which $V_0=\infty$. We need only observe what happens when we take V_0 greater and greater without limit, E_0 being left unchanged. It results that the magnitude of the transmitted wave packet (measured in any convenient way) becomes smaller and smaller, and vanishes in the limit. Thus, in the limit the wave function is identically zero on the far side of the barrier, so we have perfect reflection. It is interesting to observe that the perfect reflection is explained simply by the vanishing of the magnitude of the transmitted packet, and not by the packet suffering an infinite delay.