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Quantum Theory  
Part III

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## PART III

# APPLICATIONS TO SIMPLE SYSTEMS. FURTHER EXTENSIONS OF QUANTUM THEORY FORMULATION

## CHAPTER 11

### Solutions of Wave Equation for Square Potentials

1. Introduction to Part III. We shall apply in Part III, the physical ideas developed in Part I and the mathematical ideas developed in Part II to the solution of various elementary problems, starting from the simplest cases and gradually working up to more complex systems. We shall begin with a one-dimensional problem in which space is divided into a finite number of regions, in each of which the potential is constant but different in value from the potential of the others. With this simple problem we will be able to illustrate many important specifically quantum-mechanical effects, such as penetration of a potential barrier, reflection of electron waves by a sharp change in potential, and the binding of particles into a narrow region by an attractive force.

The next problem will be to show how Schrödinger's equation leads to results approaching those of classical physics in the correspondence limit of high quantum numbers. This will be done with the aid of the WKB approximation (Wentzel-Kramers-Brillouin). In this problem, we shall see more clearly the precise connection between classical and quantum theory. Applications of this approximation will also be made to the problem of the lifetime of excited states of a nucleus.

Throughout this treatment an effort will be made to give a simple and pictorial method for thinking of the qualitative effect of various kinds of forces on the wave function. In this way, it is hoped that the student can learn to make a qualitative picture enabling him to estimate the general form of the wave function in more complex problems, without actually solving the equations exactly. In the simple cases of the harmonic oscillator and the hydrogen atom, we shall compare the approximate results with the exact solutions.

Finally, we shall introduce the matrix formulation of quantum theory, and apply it to the case of electron spin.

2. **Eigenfunctions of the Energy.** Analogy to Index of Refraction in Optics. In Chap. 10, Sec. 35, it was shown that solutions of Schrödinger's equation which are eigenfunctions of the Hamiltonian operator are particularly significant, not only because many systems met with in practice do have a definite energy, but also because the time variation of these eigenfunctions takes the particularly simple form

$$\psi = \psi_E(x) \exp\left(-\frac{iEt}{\hbar}\right) \quad (1)$$

When a system has a definite energy, all probabilities are constant, so that the state is stationary. Furthermore, an arbitrary solution of Schrödinger's equation can be formed from suitable linear combinations of the above solutions.

In Part III, we shall concern ourselves mainly with the problem of calculating the eigenfunctions of the Hamiltonian operator. In other words, we wish to solve the equation

$$H\psi = \frac{-\hbar^2}{2m} \nabla^2 \psi + V(x)\psi = E\psi$$

and in so doing find out which values of  $E$  are permissible, in that the associated  $\psi_E$  satisfies all boundary conditions that we place on the wave function.

We may write our equation as follows:

$$\nabla^2 \psi + \frac{2m}{\hbar^2} [E - V(x)]\psi = 0 \quad (2)$$

In optics, the wave equation for a wave of definite angular frequency  $\omega$  may be written

$$\nabla^2 A + \frac{\omega^2}{c^2} n^2 A = 0 \quad (3)$$

where  $n$  is the index of refraction. Hence the wave equation for  $\psi$  now resembles that for light in a medium in which

$$n^2 = \frac{2m}{\hbar^2} [E - V(x)] \frac{c^2}{\omega^2} \quad (4)$$

or, in other words, a medium in which  $n$  is a function of the position. This is a very useful analogy, and one which we shall frequently find occasion to apply.

3. **Square Potentials.** In general,  $V(x)$  may take any conceivable functional form. A form which leads to equations that are particularly easy to solve is to have  $V$  constant everywhere in a certain region (say, from  $x = a$  to  $x = b$ ), then to have it equal to another value in the next region (say, from  $x = b$  to  $x = c$ ), then to still another value in the next

region, etc. Such a potential might look like the graph shown in Fig. 1. It is called a "square potential," because of the appearance of square corners in its graph. In nature there are no potentials which are actually square, for these imply an infinite force at the points of discontinuity in the potential. Yet, the square potential represents many actual systems roughly, and its mathematical simplicity enables us to use it to draw

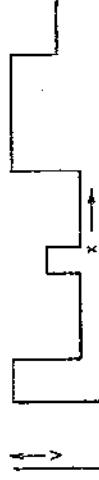


Fig. 1

conclusions that are at least qualitatively applicable to such systems. For example, the mutual potential energy of two molecules has the general form shown in Fig. 2. Many properties of molecular wave functions can be understood qualitatively by means of the square potential shown in Fig. 3, which includes two essential properties of the force; namely, attraction when the molecules are at a moderate distance, and repulsion when they are very close. It must be noted, however, that those properties of the molecule which depend on the precise shape of the curve in

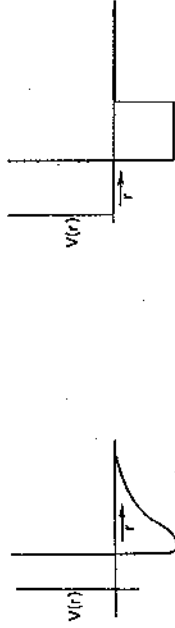


Fig. 2

Fig. 2 (for example, coefficient of thermal expansion) cannot be treated at all by this simplified potential. On the other hand, this method will give a rough approximation to the energy levels.

Another set of forces which may be represented fairly well by the square potential is the force between nuclear particles, such as neutrons and protons. The force between a proton and a neutron, for example, is characterized by two properties:

- (1) It is appreciable only over a very short distance, of the order of  $2 \times 10^{-13}$  cm. That this is indeed small can be seen by comparing it with atomic radii, which are of the order of  $2 \times 10^{-8}$  cm.
- (2) In the range where the forces are appreciable, they are very large—much larger than the forces holding atoms together.

From scattering experiments, one can get a rough idea of the shape of the potential energy of interaction between a neutron and a proton.\*

\* See Chap. 21, Sec. 56. See also H. Bethe, *Elementary Nuclear Theory*. New York: John Wiley & Sons, Inc., 1947; Chap. 4.

It is more or less as shown in Fig. 4. To a first approximation, however, the potential may be represented by the square potential of Fig. 5. The range of the potential turns out to be  $2.8 \times 10^{-13}$  cm and the depth about 20 mev. This depth contrasts with molecular interaction energies of the order of 2 ev.

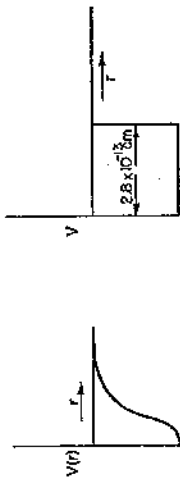


FIG. 4

**4. Solution of Problem of Square Potential.** In any region where  $V$  is constant, the solution of the wave equation is

$$\psi_x = A \exp \left[ i \sqrt{2m(E - V)} \frac{x}{\hbar} \right] + B \exp \left[ -i \sqrt{2m(E - V)} \frac{x}{\hbar} \right] \quad (5)$$

where  $A$  and  $B$  are arbitrary constants. The time-dependent solution is

$$\psi = A \exp \left[ \frac{i(px - Et)}{\hbar} \right] + B \exp \left[ \frac{-i(px + Et)}{\hbar} \right] \quad (6)$$

where  $p = \sqrt{2m(E - V)}$ . It is clear that the first term represents a wave moving to the right, while the second term represents a wave moving to the left.

As we go from one region to the next,  $V$  changes, so that the length of the wave also changes. At the boundary between regions, certain boundary conditions must be satisfied. Because the differential equation is of second order in  $x$ , it is necessary that both  $\psi$  and its first derivative be continuous at the boundaries. This follows from the fact that  $\psi$ ,  $E$ , and  $V$  are all assumed to be finite.  $\psi$  must be finite if its physical interpretation in terms of probability is to have meaning, whereas  $E$  and  $V$  must be finite, because infinite energies do not occur in nature. From the differential eq. (2), we then conclude that  $d^2\psi/dx^2$  is everywhere finite (but not necessarily continuous).  $d^2\psi/dx^2$  can be finite, however, only if  $d\psi/dx$  is continuous. Thus, we obtain the first of our boundary conditions. In order that  $d\psi/dx$  exist everywhere, however, as is implied by the mere use of a differential equation, it is also necessary that  $\psi$  be continuous. This gives us the second boundary condition.

Let us illustrate the application of these boundary conditions with the aid of a simple problem in which the potential undergoes only one discontinuous change, as shown in Fig. 6.

**Case A: ( $E > V$ )**

Suppose that electrons with some energy  $E$  are sent in from the left and that  $E > V$ . Classically we should expect that no electrons would be reflected at  $x = 0$ , since all of them have enough energy to enter the region  $x > 0$ . What is predicted by quantum theory for this problem? To answer this question, let us use the optical analogy. The electron acts, to some extent, like a wave coming in from the left, striking a sudden shift in potential at  $x = 0$ , where it experiences what is effectively a sudden shift in index of refraction. Just as with light striking a sheet of glass, we may expect part of the wave to be reflected and part to be transmitted.

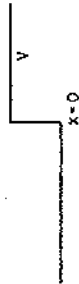


FIG. 6

In a complete quantum treatment of this problem we would actually have to start with an incident wave packet, representing the electron coming in initially from the left. This packet would come up to the barrier and part of it would be reflected and part transmitted. The reflected part of the wave packet would yield the probability that the electron was reflected, while the transmitted part would yield the probability that the electron was transmitted. We shall actually carry out this procedure in Sec. 17. Meanwhile, however, we shall adopt a procedure that is more abstract, but which leads to the same results in a mathematically simpler way. We shall assume that the packet is so broad that the incident wave can be approximated by the wave function  $B \exp(ip_1x/\hbar)$  where  $p_1 = \sqrt{2mE}$ . The incident wave will then represent a situation in which the probability density remains constant with time, but in which there is a steady stream of electrons moving to the right. The mean probability current density will be  $j = |E|^2 p_1/m$ . (In order to maintain a constant probability despite this flow of current, it would be necessary to supply electrons from the left at a steady rate.) There will also be a reflected wave, which we represent by

$$C \exp(-ip_1x/\hbar)$$

The complete wave function to the left of the barrier is

$$\psi_1 = B \exp\left(\frac{ip_1x}{\hbar}\right) + C \exp\left(\frac{-ip_1x}{\hbar}\right)$$

The transmitted wave amplitude is denoted by

$$\psi_2 = A \exp\left(\frac{-ip_2x}{\hbar}\right) \quad \text{where} \quad p_2 = \sqrt{2m(E - V)}$$

The constants  $A$ ,  $B$ , and  $C$  must now be determined from the boundary conditions that the wave function and its first derivative are continuous at  $x = 0$ .

Noting that

$$\frac{d\psi_2}{dx} = \frac{i p_2}{\hbar} A \exp\left(\frac{i p_2 x}{\hbar}\right)$$

$$\text{and } \frac{d\psi_1}{dx} = \frac{i p_1}{\hbar} \left[ B \exp\left(\frac{i p_1 x}{\hbar}\right) - C \exp\left(\frac{-i p_1 x}{\hbar}\right) \right]$$

we obtain, by setting  $x = 0$ ,

$$A = B + C \quad (7)$$

$$p_2 A = p_1(B - C) \quad (8)$$

Solution for  $A$  and  $C$  yields

$$A = \frac{2p_1 B}{p_1 + p_2} \quad (9)$$

$$C = \frac{(p_2 - p_1) B}{p_1 + p_2} \quad (10)$$

We have thus obtained the amplitudes of the reflected and transmitted waves, which are respectively  $A$  and  $C$ , in terms of  $B$ , the amplitude of the incident wave. The fraction of electrons which are transmitted,  $T$ , is equal to the ratio of the transmitted current to the incident current. The transmissivity is therefore

$$T = \frac{|A|^2 p_2}{|B|^2 p_1} = \frac{4p_1 p_2}{(p_1 + p_2)^2} \quad (11)$$

The reflectivity,  $R$ , is then just the ratio of the intensities of reflected and incident waves

$$R = \frac{|C|^2}{|B|^2} = \frac{(p_1 - p_2)^2}{(p_1 + p_2)^2} \quad (12)$$

The sum of the reflectivity and transmissivity ought, by definition, to be unity. To verify that it is, we write

$$T + R = \frac{(p_1 - p_2)^2 + 4p_1 p_2}{(p_1 + p_2)^2} = \frac{(p_1 + p_2)^2}{(p_1 + p_2)^2} = 1 \quad (13)$$

**Problem 1:** Compute the probability current for this problem (a) when  $x < 0$ , (b) when  $x > 0$ . Show that the two are the same, and thus prove that probability is conserved. Show that the current is  $S = v\rho$ , where  $v$  is the velocity of the transmitted particles,  $\rho$  is the probability density for this wave.

**Problem 2:** Show that the continuity of  $\psi$  and its derivative implies the conservation of probability current at  $x = 0$ .

We note that the reflectivity approaches zero as  $p_2$  approaches  $p_1$ , but that it approaches unity as  $p_2$  approaches zero. Since

$$p_2 = \sqrt{2m(E - V)}$$

the reflection coefficient becomes large only when  $V$  is comparable in size with  $E$ . Yet, some reflection exists no matter how small  $V$  is.

It must be emphasized again that this property of reflection from a sharp change in potential is a purely quantum-mechanical effect; it arises from the wave nature of matter and does not exist in classical theory. We shall see later, in studying the WKB approximation,\* that if the change in potential is not sharp within a wavelength of the electron wave, there will be practically no reflection. The classical result will therefore be right only in a slowly changing potential. As soon as the potential begins to change appreciably within an electron wavelength,  $\lambda = h/p$ , the wave properties of matter begin to manifest themselves, and one of them is this property of reflection from a potential that is not great enough in numerical value to stop the particle and turn it around.

*Case B: ( $E < V$ )*

If electrons are sent into this system with  $E < V$ , then according to classical physics, they will all be turned around at  $x = 0$  and none will ever penetrate to positive values of  $x$ . What does quantum theory say about this problem?

To study this question, we begin by investigating the nature of the solutions of the wave equation when  $E < V$ . In this region, the wave equation is

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + (V - E)\psi = 0$$

and the solution is

$$\psi = A \exp\left(\sqrt{2m(V - E)} \frac{x}{\hbar}\right) + B \exp\left(-\sqrt{2m(V - E)} \frac{x}{\hbar}\right) \quad (14)$$

Note that the solutions are *real* exponentials rather than complex exponentials. In order that the probability remain finite as  $x \rightarrow \infty$ , it is necessary that we choose only the negative exponential, i.e., that we choose  $A = 0$ .

When  $x < 0$ , we do as before and write the most general solution as

$$\psi = C \exp\left(i\sqrt{2mE} \frac{x}{\hbar}\right) + D \exp\left(-i\sqrt{2mE} \frac{x}{\hbar}\right) \quad (14a)$$

If the function is to be continuous at  $x = 0$ , we must have

$$C + D = B \quad (15)$$

If the derivative of  $\psi$  is to be continuous at  $x = 0$ , it is readily verified that

$$i\sqrt{2mE}(C - D) = -\frac{B}{\hbar} \sqrt{2m(V - E)}$$

or

$$C - D = iB \sqrt{\frac{V - E}{E}}$$

\* Chap. 12.

Hence, we obtain

$$C = \frac{B}{2} \left( 1 + i \sqrt{\frac{V-E}{E}} \right) \quad (16)$$

$$D = \frac{B}{2} \left( 1 - i \sqrt{\frac{V-E}{E}} \right) \quad (17)$$

The ratio of the intensity of the reflected wave to that of the incident wave is

$$R = \frac{|D|^2}{|C|^2} = 1 \quad (18)$$

It is also of interest to calculate the phase of the waves. To do this, we write  $\sqrt{(V-E)/E} = \tan \varphi$ . Then we have

$$C = \frac{B}{2} (1 + i \tan \varphi) = \frac{B}{2 \cos \varphi} (\cos \varphi + i \sin \varphi) = \frac{B}{2 \cos \varphi} e^{i\varphi} \quad (19)$$

$$D = \frac{B}{2} (1 - i \tan \varphi) = \frac{B}{2 \cos \varphi} (\cos \varphi - i \sin \varphi) = \frac{B}{2 \cos \varphi} e^{-i\varphi} \quad (20)$$

Writing

$$\frac{B}{2 \cos \varphi} = \frac{I}{2} = \text{a new constant}$$

we obtain for the wave function when  $x < 0$ ,

$$\begin{aligned} \psi &= \frac{I}{2} \left[ \exp \left( i \sqrt{2mE} \frac{x}{\hbar} + i\varphi \right) + \exp \left( -i \sqrt{2mE} \frac{x}{\hbar} - i\varphi \right) \right] \\ &= I \cos \left( \sqrt{2mE} \frac{x}{\hbar} + \varphi \right) \end{aligned} \quad (21)$$

For a typical case, the wave function looks more or less like Fig. 7.

We see from eq. (18) that the entire wave is reflected because the reflected intensity is equal to the incident intensity. Because the wave

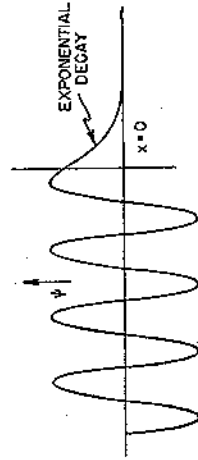


FIG. 7

equation implies the conservation of probability, we conclude that no electrons are transmitted.

**Problem 3:** Prove that the probability current is zero for Case B, that is, for  $E < V$ .

This result is in agreement with the classical prediction for this case. Yet there is a new feature, not present in the classical theory, coming from the penetration of the exponentially decaying part of the wave function into the region  $x > 0$ . This implies that an electron can be found in the region where  $V > E$ , whereas classically it could never enter this region, because it does not have enough energy.

To understand this phenomenon, we must remember that matter is not identical with the classical particle model, but that the electron also has wave properties, which can be just as important as the particle properties (see Chap. 6, Sec. 11). The region where  $V > E$  corresponds to an imaginary index of refraction

$$n^2 = \left( \frac{2m}{\hbar^2} \right) (E - V) \frac{c^2}{\omega^2}$$

We already know of one case in optics where  $n$  is imaginary, namely that of total internal reflection of light. In this case there is exactly the same type of exponential penetration of the wave from the more dense into the less dense medium.\* This new property of penetration into classically inaccessible regions must therefore be thought of in terms of the wave model; it is really one effect for which the particle model gives no description at all.

Suppose that we set up a device in the classically inaccessible region which actually measures the position of the electron; for example, we might use a microscope. Would this not involve a contradiction with the law of conservation of energy, since we would have in this region a particle with negative kinetic energy? Actually, we would find that to do an experiment which proved that the electron was definitely in this region, we would have to use such energetic light that the electron would be given a positive kinetic energy, and no contradiction would then arise from its being present in this region. To prove this, we note that any observation which guaranteed that the electron was in the region where  $V > E$  would have to put the electron into such a state that the wave function was represented by a wave packet, practically all of which was in the region where  $V > E$ . But to form a wave packet, we need wave functions that oscillate; otherwise, they cannot interfere destructively far from the center of the packet. The solutions with  $V > E$  are real exponentials in the region  $x > 0$ , so that they do not oscillate and no wave packet can be made from them. The only wave functions that oscillate are those for which  $E > V$ . We conclude that if the electron is ever in a state in which it is certain to be in the region  $x > 0$ , then it must have been given so much energy that it could have gotten into this region even classically.

\* J. A. Stratton, *Electromagnetic Theory*. New York: McGraw-Hill Book Company, Inc., 1941, p. 497.

The penetration of the electron into regions where  $V > E$  is paradoxical only if we try to hold onto the idea that matter consists of classical particles. Because of the wave properties of matter, however, an electron of definite energy is a different sort of thing from what it is classically. In fact, an electron can have a definite energy only when its wave function is an eigenfunction of the Hamiltonian operator, and therefore only when the electron is spread over a broad region of space. The electronic kinetic energy is just such a property that it must become positive whenever the electron is localized in a definite region. The statement that a particle penetrates into regions of negative kinetic energy is therefore meaningless, since the electron cannot have the localizability that leads us to attribute to it particle-like properties when it is in a region which would classically lead to negative kinetic energies. It would be just as wrong to talk of particles of negative kinetic energy as to talk of interference of particles in a Davisson-Germer experiment. Instead, we must say that both of these effects result from situations in which the wavelike aspects of matter are emphasized. In fact, from the point of view expressed in Chap. 6, Secs. 4 to 9, the process of measurement of position literally transforms the electron from a wave-like object into a particle-like object. In other words, interaction with a potential for which  $V > E$  leads to a fuller realization of the electron's wave-like potentialities, while interaction with a position-measuring device leads to a fuller realization of its particle-like potentialities.

**5. Penetration of a Barrier.** Are there any cases in which the penetration of the particle into a classically inaccessible region produces physically important results? The answer is that if the region where  $V > E$  is only of finite extent, then a particle may "leak" through a potential barrier which is so high that it could never get through classically. Suppose, for example, that the potential looked like that shown in Fig. 8.

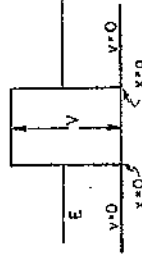


FIG. 8

In the region from  $x = 0$  to  $x = a$ ,  $V > E$ . According to classical theory, a stream of particles coming from the left would therefore be totally reflected. However, because of the wave nature of matter, we know that there is some probability that the particle penetrates out to the other side of the barrier and, as we shall show, it can actually escape into the region  $x > a$ , where  $E > V$ .

To treat this problem, we start from the right-hand side of the barrier,  $x > a$ . We know that there are no particles coming in from the right, but that there are particles streaming from the barrier toward the right. The wave function in this region is, therefore,

$$\psi = A \exp\left(\frac{i p_1 x}{\hbar}\right) \quad \text{where} \quad p_1 = \sqrt{2mE} \quad (22)$$

Within the barrier, the most general solution is

$$\psi = B \exp\left(\frac{p_2 x}{\hbar}\right) + C \exp\left(-\frac{p_2 x}{\hbar}\right) \quad \text{where} \quad p_2 = \sqrt{2m(V - E)} \quad (23)$$

We note that there is no reason now to throw out the exponentially increasing solution, because the region where  $V > E$  has only a finite extent. To make  $\psi$  and  $d\psi/dx$  continuous at  $x = a$ , we must have

$$B \exp\left(\frac{p_2 a}{\hbar}\right) + C \exp\left(-\frac{p_2 a}{\hbar}\right) = A \exp\left(\frac{i p_1 a}{\hbar}\right) \quad (24)$$

$$B \exp\left(\frac{p_2 a}{\hbar}\right) - C \exp\left(-\frac{p_2 a}{\hbar}\right) = \frac{A i p_1}{p_2} \exp\left(\frac{i p_1 a}{\hbar}\right) \quad (25)$$

Solving for  $B$  and  $C$ , we get

$$B = \frac{A}{2} \left(1 + \frac{i p_1}{p_2}\right) \exp\left[\frac{i p_1 (a - p_2)}{\hbar}\right] \quad (26)$$

$$C = \frac{A}{2} \left(1 - \frac{i p_1}{p_2}\right) \exp\left[\frac{i p_1 (a + p_2)}{\hbar}\right] \quad (27)$$

Let us consider the case where  $p_2 a / \hbar \gg 1$ ; in other words, we suppose that the exponentials change a great deal from one side of the barrier to the other. We then notice that  $|C| \gg |B|$ . At the other side of the barrier (where  $x = 0$ ), the main term in the wave function is the one involving  $C \exp(-p_2 x / \hbar)$ .

When  $x < 0$ , the wave function is

$$\psi = D \exp\left(\frac{i p_1 x}{\hbar}\right) + E \exp\left(-\frac{i p_1 x}{\hbar}\right) \quad (28)$$

In order that  $\psi$  and  $\partial\psi/\partial x$  be continuous at  $x = 0$ , we must have

$$D + E = C + B \quad (29)$$

$$D - E = \frac{i p_2}{p_1} (C - B) \quad (30)$$

$$D = \frac{C}{2} \left(1 + \frac{i p_2}{p_1}\right) + \frac{B}{2} \left(1 - \frac{i p_2}{p_1}\right) \quad (31)$$

$$E = \frac{C}{2} \left(1 - \frac{i p_2}{p_1}\right) + \frac{B}{2} \left(1 + \frac{i p_2}{p_1}\right) \quad (32)$$

If the barrier is thick, we may, to a first approximation, neglect  $B$ . We then obtain

$$D = \frac{A}{4} \left(1 + \frac{i p_2}{p_1}\right) \left(1 - \frac{i p_1}{p_2}\right) \exp\left(\frac{i p_1 a}{\hbar}\right) \exp\left(\frac{p_2 a}{\hbar}\right) \quad (33)$$

$$E = \frac{A}{4} \left(1 - \frac{i p_2}{p_1}\right) \left(1 - \frac{i p_1}{p_2}\right) \exp\left(\frac{i p_1 a}{\hbar}\right) \exp\left(\frac{p_2 a}{\hbar}\right) \quad (34)$$

It is of interest to solve for the ratio of the intensity of the transmitted wave to that of the incident wave, i.e., the transmission coefficient  $T$ .

$$T = \frac{|A|^2}{|D|^2} = \frac{16 \exp(-2p_2 a / \hbar)}{[1 + (p_2/p_1)^2][1 + (p_1/p_2)^2]} \quad (34)$$

The preceding result shows that there is a small probability that an object can penetrate a potential barrier which it could not even enter according to classical theory. This probability decreases rapidly as the barrier gets thicker and also as it gets higher.

As pointed out in Sec. 4, this property of barrier penetration is entirely due to the wave aspects of matter and is, in fact, very similar to the total internal reflection of light waves. If two slabs of glass are placed close to each other, but not touching, then light will be transmitted from one

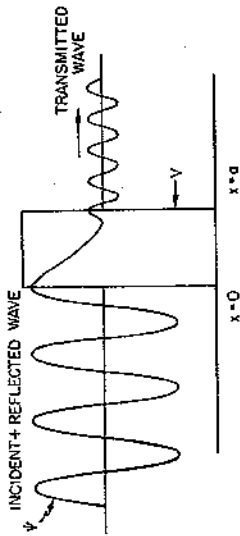


Fig. 9

slab to the second, even if the angle of incidence is greater than the critical angle. The intensity of the transmitted wave, however, decreases exponentially with the thickness of the layer of air. The reason for the transmission is exactly the same as with electron waves, namely, the exponential penetration of the wave into the region of imaginary index of refraction.

The wave function looks more or less as in Fig. 9. Most of the incident wave is reflected, but a small part is transmitted.

In order to compute the reflection coefficient, it is necessary to use the exact solution, which does not neglect  $B$ . The reflection coefficient is

$$R = \frac{|E|^2}{|D|^2} \quad (35)$$

**Problem 4:** Prove (with the exact solution) that  $T + R = 1$ .

Compute the probability current inside the barrier and show that it is equal to the current in the transmitted wave. Hence verify the conservation of probability for this case. (Note that the current for this case is contributed to by the effects of interference of the exponentially increasing and exponentially decreasing solutions. As a result, the neglect of the smaller solution in this region is not permitted if we wish to compute the current.)

**6. Applications of Barrier Penetration.** The principal example of barrier penetration is the  $\alpha$  decay of nuclei. It is known that certain

nuclei can emit  $\alpha$  particles, but the mean time needed to emit such particles varies over an enormous range from one radioactive nucleus to another. The theory of  $\alpha$  decay is based on the idea that the  $\alpha$  particles are held inside the nucleus by tremendous attractive forces, very similar to those involved in the attraction of neutrons for protons. These forces, however, have a very short range, so that they are completely negligible unless the  $\alpha$  particle is inside the nucleus. The  $\alpha$  particles and the nucleus are both positively charged. This means that the electrical forces tend to make them repel each other. When the  $\alpha$  particle is inside the nucleus, this electrical repulsion is much less than the nuclear attractive forces, but outside the nucleus it is the only force present. If, therefore, an  $\alpha$  particle is brought toward a nucleus from a long distance, it will at first be repelled electrically and will have a potential energy

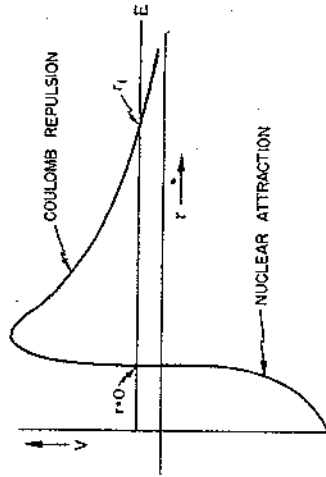


Fig. 10

$2Ze^2/r$ , where  $Ze$  is the charge on the nucleus and  $2e$  is the charge on the  $\alpha$  particle. When it reaches the nucleus, this repulsion is rapidly overbalanced by the nuclear attraction. The potential curve as a function of the distance  $r$  of the  $\alpha$  particle from the center of the nucleus looks more or less like the curve shown in Fig. 10. If the  $\alpha$  particle has an energy  $E$  that is not great enough to carry it over the repulsive Coulomb barrier, then, according to classical physics, the  $\alpha$  particle would be trapped inside the nucleus, once it got in. But because of its wave properties, the  $\alpha$  particle actually has a small probability of leaking through the barrier.

To find the mean rate of emission, we assume that the  $\alpha$  particle moves back and forth more or less freely inside the nucleus. There is independent evidence that it does so at a speed of about  $10^9$  cm/sec.\* Since the heavy radioactive nuclei, such as uranium, have radii of about  $10^{-12}$  cm, the  $\alpha$  particle strikes the barrier about  $10^{21}$  times per second. Each time it strikes the barrier, the probability that it penetrates is equal to

\* H. Bethe, *Elementary Nuclear Physics*, p. 110.

the transmissivity  $T$ , of the barrier, given by eq. (34). Hence, the probability that it comes out in one second is given by

$$P = 10^{21}T \quad \text{per sec}$$

The mean lifetime of the nucleus is just the reciprocal of this, or

$$\tau = \frac{10^{-21}}{T} \quad \text{sec}$$

To compute  $T$ , we need to know the quantities  $E - V$  and  $a$ , the thickness of the barrier. Actually, the barrier is far from rectangular, as can be seen from Fig. 4; hence, the present treatment is not very good for this case. A better treatment will be given later with the aid of the WKB approximation. Here we shall merely attempt to obtain an order of magnitude for  $T$ . For uranium, the mean value of  $V - E$  is about 12 mev,\* the mean width about  $3 \times 10^{-12}$  cm.

The factor  $[1 + (p_2/p_1)^2][1 + (p_1/p_2)^2]$  is so close to unity that we can neglect it in comparison with the exponential. For the  $\alpha$  particle,  $m = 6.4 \times 10^{-24}$  gram. Noting that 1 ev =  $1.6 \times 10^{-12}$  ergs, we obtain

$$\begin{aligned} 2\sqrt{2m(V-E)}\frac{a}{\hbar} &= \frac{2\sqrt{12.8 \times 10^{-24} \times 12 \times 1.6 \times 10^{-12}}}{1.07 \times 10^{-27}} \times 3 \times 10^{-12} \cong 90 \end{aligned}$$

The result is that

$$P = 10^{21} e^{-90} = 10^{-15} \text{ per sec} = 10^{-11} \text{ per year}$$

It is clear that this number is sensitive to the exact value of  $(V - E)$  and  $a$ , since these appear in the exponential. As a result this treatment gives merely a crude estimate. We can also see that the lifetimes for different elements may be expected to vary widely, since  $V - E$  and  $a$  will vary, and since the exponential is sensitive to these quantities. In Chap. 12, however, with the aid of the WKB approximation, we shall give a treatment that is in closer agreement with experiment and that gives a better idea of how the lifetime for a decay varies for different elements.

7. **The Square Well Potential.** Let us now consider a square potential that is attractive, rather than repulsive, as shown in Fig. 11. Let this potential be  $-V_0$  in the region from  $x = a$  to  $x = -a$ , and zero elsewhere. Now, suppose that a stream of electrons is directed at it from the left. According to classical physics, no electrons would ever be turned back but, as we have already seen, the wave theory tells us that electrons will be reflected from the sharp edges at  $x = a$  and  $x = -a$ .

\* H. Bethe, *Elementary Nuclear Physics*.

As a result, there will be a reflected and a transmitted wave, as well as an incident wave.\*

To solve this problem, we start in the region  $x > a$ , where there is only a transmitted wave. The wave function is, therefore,

$$\psi = A \exp\left(\frac{ip_1x}{\hbar}\right) \quad (36)$$

where  $p_1$  is the momentum in the region

$$p_1 = \sqrt{2mE}$$

In the region of the well, from  $x = -a$  to  $x = +a$ , the wave function is

$$\psi = B \exp\left(\frac{ip_2x}{\hbar}\right) + C \exp\left(-\frac{ip_2x}{\hbar}\right) \quad (37)$$

where  $p_2 = \sqrt{2m(E + V_0)}$ .

To solve for  $B$  and  $C$  in terms of  $A$ , we must make  $\psi$  and  $d\psi/dx$  continuous at  $x = a$ :

$$A \exp\left(\frac{ip_1a}{\hbar}\right) = B \exp\left(\frac{ip_2a}{\hbar}\right) + C \exp\left(-\frac{ip_2a}{\hbar}\right) \quad (38)$$

$$\frac{p_1}{p_2} A \exp\left(\frac{ip_1a}{\hbar}\right) = B \exp\left(\frac{ip_2a}{\hbar}\right) - C \exp\left(-\frac{ip_2a}{\hbar}\right) \quad (39)$$

Solution of these equations yields

$$B = \frac{A}{2} \left(1 + \frac{p_1}{p_2}\right) \exp\left[\frac{i(p_1 - p_2)a}{\hbar}\right] \quad (40)$$

$$C = \frac{A}{2} \left(1 - \frac{p_1}{p_2}\right) \exp\left[\frac{i(p_1 + p_2)a}{\hbar}\right] \quad (41)$$

In the region  $x < -a$ , the wave function is

$$\psi = D \exp\left(\frac{ip_1x}{\hbar}\right) + E \exp\left(-\frac{ip_1x}{\hbar}\right) \quad (42)$$

To make  $\psi$  and  $d\psi/dx$  continuous at  $x = -a$ , we have

$$\begin{aligned} D \exp\left(-\frac{ip_1a}{\hbar}\right) + E \exp\left(\frac{ip_1a}{\hbar}\right) &= B \exp\left(-\frac{ip_2a}{\hbar}\right) + C \exp\left(\frac{ip_2a}{\hbar}\right) \quad (43) \end{aligned}$$

\* Note that this treatment will also apply to the potential barrier, provided that  $E > V_0$ , i.e., provided that the kinetic energy inside the barrier remains positive.

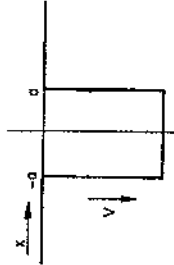


FIG. 11



$$D \exp\left(-\frac{ip_1 a}{\hbar}\right) - E \exp\left(\frac{ip_1 a}{\hbar}\right) = \left(\frac{p_2}{p_1}\right) \left[ B \exp\left(-\frac{ip_2 a}{\hbar}\right) - C \exp\left(\frac{ip_2 a}{\hbar}\right) \right] \quad (44)$$

$$D = \left(\frac{B}{2}\right) \left(1 + \frac{p_2}{p_1}\right) \exp\left[\frac{i(p_1 - p_2)a}{\hbar}\right] + \left(\frac{C}{2}\right) \left(1 - \frac{p_2}{p_1}\right) \exp\left[\frac{i(p_1 + p_2)a}{\hbar}\right] \quad (45)$$

$$E = \left(\frac{B}{2}\right) \left(1 - \frac{p_2}{p_1}\right) \exp\left[-\frac{i(p_1 + p_2)a}{\hbar}\right] + \left(\frac{C}{2}\right) \left(1 + \frac{p_2}{p_1}\right) \exp\left[\frac{i(p_2 - p_1)a}{\hbar}\right] \quad (46)$$

$$D = \left(\frac{A}{4}\right) \exp\left(\frac{2ip_1 a}{\hbar}\right) \left[ \left(1 + \frac{p_2}{p_1}\right) \left(1 + \frac{p_1}{p_2}\right) \exp\left(-\frac{2ip_2 a}{\hbar}\right) + \left(1 - \frac{p_2}{p_1}\right) \left(1 - \frac{p_1}{p_2}\right) \exp\left(\frac{2ip_2 a}{\hbar}\right) \right] \quad (47)$$

$$E = \left(\frac{A}{4}\right) \left[ \left(1 - \frac{p_2}{p_1}\right) \left(1 + \frac{p_1}{p_2}\right) \exp\left(-\frac{2ip_2 a}{\hbar}\right) + \left(1 + \frac{p_2}{p_1}\right) \left(1 - \frac{p_1}{p_2}\right) \exp\left(\frac{2ip_2 a}{\hbar}\right) \right] \quad (48)$$

The transmissivity is

$$T = \frac{|A|^2}{|D|^2} = \left[ \cos\left(\frac{2p_2 a}{\hbar}\right) + \frac{i}{2} \left(\frac{p_1}{p_2} + \frac{p_2}{p_1}\right) \sin\left(\frac{2p_2 a}{\hbar}\right) \right]^{-2} = \left[ \cos^2\left(\frac{2p_2 a}{\hbar}\right) + \frac{1}{4} \left(\frac{p_1}{p_2} + \frac{p_2}{p_1}\right)^2 \sin^2\left(\frac{2p_2 a}{\hbar}\right) \right]^{-1} \quad (49)$$

Noting that

$$\cos^2 = 1 - \sin^2 \quad \text{and} \quad \left(\frac{p_1}{p_2} + \frac{p_2}{p_1}\right)^2 - 4 = \left(\frac{p_1}{p_2} - \frac{p_2}{p_1}\right)^2$$

we obtain

$$T = \frac{1}{1 + \frac{1}{4} \left(\frac{p_1}{p_2} - \frac{p_2}{p_1}\right)^2 \sin^2\left(\frac{2p_2 a}{\hbar}\right)} \quad (50)$$

This result is very interesting. First, we see that for  $p_1 = p_2$ ,  $T = 1$ . This is very natural, because there is then no potential well at all. If  $p_1 \neq p_2$ , the transmissivity is, in general, less than unity, indicating that some reflection has taken place. This reflection from an attractive potential is a result of the wave nature of matter; it resembles the reflection of sound waves from the open end of an organ pipe. There is, however, one case in which  $T = 1$  even though  $p_1 \neq p_2$ , namely, when  $\sin^2(2p_2 a/\hbar) = 0$ , or  $p_2 = N\pi\hbar/2a$ , where  $N$  is an integer.

How can we understand this result? To see what it means, we note

that this problem is very similar to that of the Fabry-Perot interferometer in optics.\* In our problem, the wave is reflected at the sharp edges of the potential, which correspond to the edges of a piece of glass in optics, where, likewise, a sharp change of index of refraction takes place. This problem therefore resembles that of two sheets of glass, separated by a distance of  $2a$ . In the treatment of the Fabry-Perot interferometer, it is shown that if the wave, which reflects from the surface at  $x = +a$ ,



FIG. 12

arrives back at that surface after reflecting from  $x = -a$  with a phase shift of  $2\pi N$ , then it will interfere constructively with the next wave coming in and, as a result, the transmitted wave is reinforced. Thus, for certain wavelengths, the transmission coefficient is unity. As a function of wave number, the transmission coefficient resembles the curve given in Fig. 12. The sharpness and breadth of the peaks depend on the reflection coefficient and, in our problem, this depends on the ratio  $p_1/p_2$ .

Problem 5: Compute the reflectivity,  $R = |E|^2/|D|^2$  and show that  $T + R = 1$ .

8. Width of Peak in Transmission Resonances. To compute the width of the peak, we first assume that  $p_2/p_1$  is large, so that the peak will be sharp. Then we shall ask how far from  $p_2 = N\pi\hbar/2a$  we will have to be to make  $T$  drop to  $\frac{1}{2}$ . This will occur where

$$\frac{1}{4} \left(\frac{p_1}{p_2} - \frac{p_2}{p_1}\right)^2 \sin^2\left(\frac{2p_2 a}{\hbar}\right) = 1 \quad (51)$$

or where

$$\sin\left(\frac{2p_2 a}{\hbar}\right) = \pm \frac{2}{\left|\frac{p_1}{p_2} - \frac{p_2}{p_1}\right|} \quad (52)$$

If the denominator on the right is large, then  $2p_2 a/\hbar$  will differ only slightly from  $N\pi$  at this point, and we can write

$$\frac{2p_2 a}{\hbar} \cong N\pi \pm \frac{2}{\left|\frac{p_1}{p_2} - \frac{p_2}{p_1}\right|} \quad (53)$$

$$p_2 \cong \frac{N\pi\hbar}{2a} \pm \frac{\hbar/a}{\left|\frac{p_1}{p_2} - \frac{p_2}{p_1}\right|} \quad (54)$$

$$\delta p_2 \cong \frac{\hbar}{a} \frac{1}{\left|\frac{p_1}{p_2} - \frac{p_2}{p_1}\right|} \quad (55)$$

\* F. A. Jenkins and H. E. White, *Fundamentals of Physical Optics*. New York: McGraw-Hill Book Company, Inc., 1937, p. 93.

Writing  $p_2 = \sqrt{2m(E + V_0)}$ , we get, by differentiation (assuming  $\delta p_2/p_2$  to be small),

$$\delta p_2 \cong \sqrt{\frac{m}{2(E + V_0)}} \delta E \quad (55a)$$

and

$$\delta E \cong \sqrt{\frac{2(E + V_0)}{m}} \delta p_2 \cong \sqrt{\frac{2(E + V_0) \hbar}{m}} \frac{1}{a} \frac{1}{|p_1/p_2 - p_2/p_1|} = \frac{v_2 \hbar / a}{|p_1/p_2 - p_2/p_1|} \quad (56)$$

where  $v_2$  is the velocity of the particle inside the well.

It is easy to explain the width of the transmission resonances in terms of the process of reflection of the wave back and forth between the edges of the potential well. If  $T$  is the transmission coefficient for a wave striking the sharp potential edge at  $x = a$ , then the wave will reflect back and forth approximately  $1/T$  times before most of it has been transmitted. According to eq. (11), the transmission coefficient is

$$T = \frac{4p_2 p_1}{(p_1 + p_2)^2}$$

where  $p_1$  is the momentum of the transmitted particle and  $p_2$  that of the incident particle.

The phase shift suffered by a wave as it crosses the well and returns is  $4p_2 a / \hbar$ , which is equal to  $2N\pi$  for the case of exact resonance. The total phase shift after  $1/T$  reflections is  $\varphi = 4p_2 a / T \hbar$ , which is equal to  $\varphi_2 = 2N\pi / T$  for exact resonance. Constructive interference will begin to fail when  $\varphi - \varphi_2 \cong 1$ , or when

$$\varphi - \varphi_2 = \frac{4\Delta p_2 a}{T \hbar} \cong 1$$

$$\text{and} \quad \Delta p_2 \cong \frac{\hbar T}{4a} \cong \frac{p_1 p_2}{(p_1 + p_2)^2} \frac{\hbar}{a}$$

In order that a sharp resonance occur, it is necessary that  $T$  be small, so that many reflections can take place. This will happen only if  $p_1 \ll p_2$ .

As a result,  $(p_1 + p_2)^2 \cong p_2^2$ , and we obtain  $\Delta p_2 \cong \frac{p_1 \hbar}{p_2 a}$ . This is the same as obtained in eq. (55), using the same approximation, i.e.,  $p_1 \ll p_2$ . Note that the whole argument is only approximate and qualitative.

**9. The Ramsauer Effect.** An interesting example of these transmission "resonances" occurs in the scattering of electrons from atoms of noble gases, such as neon and argon. The potential energy of an electron inside such an atom looks somewhat as shown in Fig. 13. To a first approximation, it may be represented as a square well of radius about

$2 \times 10^{-8}$  cm and uniform depth  $V_0$ . Now, it turns out that for very slow electrons, having a kinetic energy of the order of 0.1 electron volt, the effective depth and radius of the well are such that there is a transmission resonance for electrons. Thus, the atom seems to be practically transparent to electrons of this speed. Also, the probability of scattering, for example, is much less than is obtained with atoms for which this resonance does not exist, or for the same atoms at higher electronic energies, for which the resonance also does not exist.

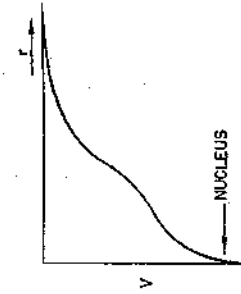


Fig. 13

This effect was first observed experimentally by Ramsauer and was later explained in terms of quantum theory. We shall study this effect in greater detail in the theory of scattering, where the complications resulting from the three-dimensional nature of the problem are taken into account.\*

**Problem 6:** Assuming a square well of range  $2 \times 10^{-8}$  cm, how deep would the well have to be to provide a transmission resonance for electrons of 0.1-ev kinetic energy?

**10. Bound States.** According to classical theory, a particle for which  $E < 0$  would be bound inside the potential well, because it would not have the energy to escape. Are there any bound states in the quantum treatment of this problem? We shall see that there may be such bound states but that, in general, the possible energies of bound states are not continuous as in classical theory, but discrete. This is also in contrast to quantum results for positive energies, where we have seen that there was no restriction on the values of  $E$  for which solutions to the wave equation existed, so that a continuous spectrum is obtained in this case.

We begin the solution for the bound-state eigenfunctions and eigenvalues by noting that in the region where  $x > a$ , the solution is a linear combination of real exponentials; hence to make  $\psi$  finite as  $x \rightarrow \infty$ , we must choose the exponential that decreases with increasing  $x$ . Thus we write  $\psi = A \exp(-p_1 x / \hbar)$ , where  $p_1 = \sqrt{2m|E|}$  and  $E$  is the energy of the bound state, which is negative.†

Within the square well, the wave function is

$$\psi = B \exp\left(\frac{ip_2 x}{\hbar}\right) + C \exp\left(-\frac{ip_2 x}{\hbar}\right) \quad (57)$$

where  $p_2 = \sqrt{2m(V_0 - |E|)}$ . The continuity conditions lead to (for  $x = a$ )

\* See Chap. 21, Sec. 51. See also N. F. Mott and H. S. W. Massey, *The Theory of Atomic Collisions*, Oxford: Clarendon Press, 1933, p. 133.

†  $V_0$  is by definition a positive number, as defined in connection with Fig. 12.

$$B \exp\left(\frac{ip_2 a}{\hbar}\right) + C \exp\left(-\frac{ip_2 a}{\hbar}\right) = A \exp\left(-\frac{p_1 a}{\hbar}\right)$$

$$B \exp\left(\frac{ip_2 a}{\hbar}\right) - C \exp\left(-\frac{ip_2 a}{\hbar}\right) = \frac{iA p_1}{p_2} \exp\left(-\frac{p_1 a}{\hbar}\right)$$

Solving for  $B$  and  $C$ , we get

$$B = \frac{A}{2} \left(1 + \frac{ip_1}{p_2}\right) \exp\left[-\frac{a}{\hbar}(p_1 + ip_2)\right]$$

$$C = \frac{A}{2} \left(1 - \frac{ip_1}{p_2}\right) \exp\left[-\frac{a}{\hbar}(p_1 - ip_2)\right]$$

It is now necessary that at  $x = -a$ , the solution fit smoothly onto an exponential which decreases as  $x \rightarrow -\infty$ . This will not happen, in general, unless the binding energy,  $|E|$ , has a suitable value. To find out when such a solution is possible, we write (for  $x < -a$ )

$$\psi = D \exp\left(\frac{p_1 x}{\hbar}\right) \quad (58)$$

The continuity conditions are

$$D \exp\left(\frac{p_1 a}{\hbar}\right) = B \exp\left(-\frac{ip_2 a}{\hbar}\right) + C \exp\left(\frac{ip_2 a}{\hbar}\right) \quad (59)$$

$$\frac{p_1}{p_2} D \exp\left(\frac{p_1 a}{\hbar}\right) = i \left[ B \exp\left(-\frac{ip_2 a}{\hbar}\right) - C \exp\left(\frac{ip_2 a}{\hbar}\right) \right] \quad (60)$$

By dividing the second of these by the first, we obtain

$$-i \frac{p_1}{p_2} = \frac{B \exp(-ip_2 a/\hbar) - C \exp(ip_2 a/\hbar)}{B \exp(-ip_2 a/\hbar) + C \exp(ip_2 a/\hbar)}$$

$$= \frac{[1 + (ip_1/p_2)] \exp(-2ip_2 a/\hbar) - [1 - (ip_1/p_2)] \exp(2ip_2 a/\hbar)}{[1 + (ip_1/p_2)] \exp(-2ip_2 a/\hbar) + [1 - (ip_1/p_2)] \exp(2ip_2 a/\hbar)}$$

To simplify this expression, we write

$$\frac{p_1}{p_2} = \tan \varphi, \quad 1 + \frac{ip_1}{p_2} = \frac{1}{\cos \varphi} (\cos \varphi + i \sin \varphi) = \frac{e^{i\varphi}}{\cos \varphi}$$

We get

$$\tan \varphi = i \frac{\exp[i(\varphi - 2p_2 a/\hbar)] - \exp[-i(\varphi - 2p_2 a/\hbar)]}{\exp[i(\varphi - 2p_2 a/\hbar)] + \exp[-i(\varphi - 2p_2 a/\hbar)]}$$

$$= \tan\left(\frac{2p_2 a}{\hbar} - \varphi\right) \quad (61)$$

The above equation implies that  $\varphi = 2p_2 a/\hbar - \varphi + N\pi$ , where  $N$  is any integer, positive or negative. Solution for  $\varphi$  yields

$$\varphi = p_2 \frac{a}{\hbar} + \frac{N\pi}{2}$$

$$\tan \varphi = \frac{p_1}{p_2} = \tan\left(\frac{p_2 a}{\hbar} + \frac{N\pi}{2}\right) = \begin{cases} \tan \frac{p_2 a}{\hbar} & N \text{ even} \\ -\cot \frac{p_2 a}{\hbar} & N \text{ odd} \end{cases} \quad (62)$$

Expressing  $p_1$  and  $p_2$  in terms of  $E$  and  $V_0$ , we then obtain

$$\sqrt{\frac{|E|}{V_0 - |E|}} = \begin{cases} \tan \left[ \frac{a}{\hbar} \sqrt{2m(V_0 - |E|)} \right] & N \text{ even} \\ -\cot \left[ \frac{a}{\hbar} \sqrt{2m(V_0 - |E|)} \right] & N \text{ odd} \end{cases} \quad (63)$$

The above is a transcendental equation defining  $|E|$ . Wherever it has a solution, we have a possible energy level. The equation must, in general, be solved numerically or graphically. We can, however, obtain an approximate idea of the location of the energy levels. To do this, we rewrite the equations with the substitution

$$\sqrt{2m(V_0 - |E|)} \frac{a}{\hbar} = \xi; \quad 2m|E| = 2mV_0 - \left(\frac{\hbar}{a}\right)^2 \xi^2 \quad (64)$$

These yield

$$\frac{\hbar}{a} \frac{\xi}{\sqrt{2mV_0 - (\hbar/a)^2 \xi^2}} = \begin{cases} \cot \xi & N \text{ even} \\ -\tan \xi & N \text{ odd} \end{cases} \quad (65)$$

After we have solved for  $\xi$ , then we can obtain  $|E|$  from eq. (64)

Case A:  $N$  odd.

It is necessary to find the intersection of the curve  $y_1 = \tan \xi$  with the curve

$$y_2 = -\frac{\hbar}{a} \xi \left[ 2mV_0 - \left(\frac{\hbar}{a}\right)^2 \xi^2 \right]^{-1/2}$$

(see Fig. 14). We note that the curve for  $y_2$  extends only as far as

$$\xi = \pm \sqrt{2mV_0} \frac{a}{\hbar}$$

since, by definition,  $|E|$  must be positive, and larger values of  $\xi$  would lead to negative values of  $|E|$  in eq. (64). The curve for  $y_2$  goes through the origin, with a slope depending on  $V_0$  and  $a$ , and finally becomes infinite at

$$\xi = \pm \sqrt{2mV_0} \frac{a}{\hbar}$$

The intersection of  $y_1$  and  $y_2$  at  $\xi = 0$  is an extraneous root and does not lead to a true solution of Schrödinger's equation.

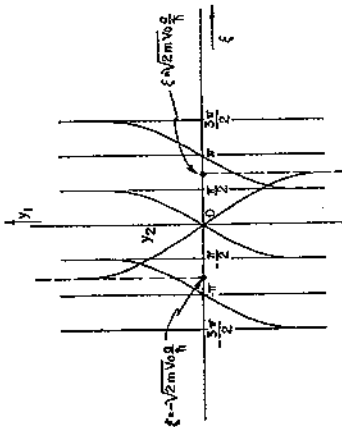


FIG. 14

**Problem 7:** Prove by substitution of eq. (57) into Schrödinger's equation that the root  $\xi = 0$  does not lead to a solution.

If  $\sqrt{2mV_0} \frac{a}{\hbar} < \frac{\pi}{2}$ , there will be no additional intersections between  $y_1$  and  $y_2$ , and therefore no bound-state solutions. It is readily verifiable that the condition for  $N$  bound-state solutions is

$$\sqrt{2mV_0} \frac{a}{\hbar} > \left(N + \frac{1}{2}\right) \pi$$

$$V_0 > \frac{1}{2m} \left(\frac{\hbar}{a}\right)^2 \left(N + \frac{1}{2}\right)^2 \pi^2$$

or

Note that we always obtain positive and negative roots in pairs. Since the value of  $|E|$  depends only on  $\xi^2$  [see eq. (64)], each pair leads, however, to only one value of  $|E|$ .

*Case B: N even.*

A similar treatment can be given for  $N$  even. We plot  $y_1 = \cot \xi$ , and find its intersection with

$$y_2 = \frac{\hbar}{a} \sqrt{2mV_0 - (\hbar/a)^2 \xi^2}$$

(see Fig. 15).

The first solution occurs when  $\xi < \pi/2$ , the next one when  $\xi > \pi$ , and so on. At least one solution of this type ( $N$  even) can therefore exist, no matter how small  $V_0$  is. For two solutions to exist, it is necessary that  $\xi > \pi$ , or that  $V_0 > \frac{1}{2m} \left(\frac{\hbar}{a}\right)^2 \pi^2$ . As  $V_0$  is increased, more and more solutions eventually become possible.

**Problem 8:** Suppose  $V_0$  is 20 mev,  $a = 2.8 \times 10^{-13}$  cm. Find the energy levels (numerically or graphically) for a proton ( $m = 1.6 \times 10^{-24}$  gram) in such a well. Find them for an  $\alpha$  particle of mass  $m = 6.4 \times 10^{-24}$  gram.

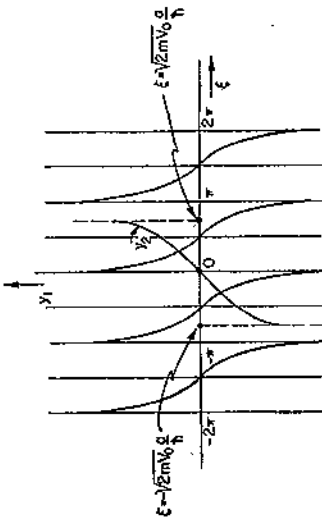


FIG. 15

**11. Limit of an Infinitely Deep Well.** If a well is infinitely deep, the solution in the classically inaccessible region,  $\exp\left[-\sqrt{2m(V_0 - |E|)} \frac{x}{\hbar}\right]$ , dies out with infinite speed, so that the wave function must be zero at each edge of the well. The solution must then be  $\psi = \sin\left(N \frac{\pi x}{2a}\right)$ , where  $N$  is any integer.\* Since the solution can also be written

$$\psi = \sin \sqrt{2m(V_0 - |E|)} \frac{x}{\hbar}$$

we have

$$\sqrt{V_0 - |E|} = \frac{\hbar}{a} \left(\frac{N\pi}{2}\right) \sqrt{2m} \quad \text{or} \quad V_0 - |E| = \frac{1}{2m} \left(\frac{\hbar}{a}\right)^2 \left(\frac{N\pi}{2}\right)^2$$

We can readily verify that eqs. (63) lead to the same solution since, as  $V_0 \rightarrow \infty$ , we have  $\frac{|E|}{V_0 - |E|} \rightarrow 0$ ; hence

$$\left. \begin{aligned} N \text{ odd:} \quad & \tan \sqrt{2m(V_0 - |E|)} \frac{a}{\hbar} \rightarrow 0 \\ N \text{ even:} \quad & \cot \sqrt{2m(V_0 - |E|)} \frac{a}{\hbar} \rightarrow 0 \end{aligned} \right\}$$

This leads to

$$\sqrt{V_0 - |E|} = \frac{1}{\sqrt{2m}} \left(\frac{\hbar}{a}\right) \frac{N\pi}{2}$$

which is in agreement with the result obtained directly.

\* We have, for convenience, shifted the origin to one side of the well. We retain this notation only in this section.

**12. Graphical Interpretation of Solutions.** There is a simple graphical point of view that enables us to understand readily the general nature of all these different kinds of solutions. Let us consider the wave equation

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}(E - V)\psi = 0. \quad (1)$$

This equation defines the second derivative of the wave function  $\psi$ , in terms of  $\psi$  and  $E - V$ . When  $E > V$  (positive kinetic energy), the second derivative is opposite in sign to  $\psi$  itself.  $\psi$  is, therefore, concave toward the axis, so that the wave function will tend to oscillate. (This result is in agreement with the exact solution

$$\psi = A \cos \sqrt{2m(E - V)} \frac{x}{\hbar} + B \sin \sqrt{2m(E - V)} \frac{x}{\hbar}$$

The bigger  $E - V$  is, the more rapidly does  $\psi$  curve, and the more rapidly it oscillates.)

When  $V > E$ , however,  $d^2\psi/dx^2$  has the same sign as  $\psi$ , so that  $\psi$  is convex toward the axis. This means that if  $\psi$  is already increasing, it will increase even more rapidly, because the slope must be always increasing. (This is in agreement with the exact solution,

$$\psi = A \exp \left[ -\sqrt{2m(V - E)} \frac{x}{\hbar} \right] + B \exp \left[ \sqrt{2m(V - E)} \frac{x}{\hbar} \right]$$

The bigger  $V - E$  is, the more rapidly will the exponential change.)

Let us now consider the bound states of the square well. When  $x < -a$  (see Fig. 16), we start with an exponential solution that is increasing with increasing  $x$  and curving upward. At  $x = -a$ , the kinetic energy becomes positive and, since  $\psi$  is positive, the curvature becomes negative. The wave function then begins to curve back toward  $\psi = 0$ , at a rate depending on  $V_0 - |E|$ . If  $V_0 - |E|$  is large enough, the slope will be negative by the time we reach  $x = a$ . When  $x > a$ , the function begins to curve back upward again, because  $V_0 - |E|$  is negative. For a general choice of  $|E|$ , it will eventually increase without bounds and, therefore, become an inadmissible solution. Only if  $|E|$  is such that the slope at  $x = a$  exactly matches the required slope of a decreasing exponential

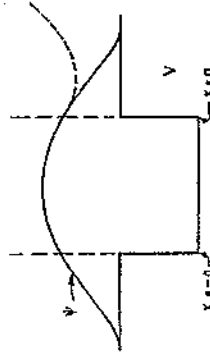


Fig. 16

$$\left[ \psi = \exp \left( -\frac{x}{\hbar} \sqrt{2m|E|} \right) \right]$$

will the solution remain bounded as  $x \rightarrow \infty$ . Thus, only certain values of  $|E|$  will lead to bound states. These will be the eigenvalues.

If  $V_0$  is very large, then  $\psi$  can fit onto the decaying exponential at  $x = a$  after one or more oscillations. These will be additional bound states. Such possibilities are illustrated in Fig. 17. The larger  $V_0$  is, the greater, in general, will be the number of such possibilities.

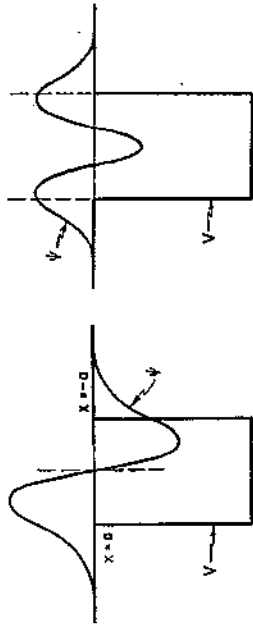


Fig. 17

Each solution may be described in terms of the number of zeros (or nodes) that the wave function has. For example, the first solution mentioned has no nodes, the second solution has one, the third two, etc. Generally, the number of nodes in the solution is equal to the number  $N$ , appearing in eq. (64).

### Solution for Wave Function

For each value of  $N$  for which there is a solution to eq. (63), we can now solve for the wave function. To do this, we note that once  $|E|$  is known,  $p_1 = \sqrt{2m|E|}$  and  $p_2 = \sqrt{2m(V_0 - |E|)}$  are also known. This means that (57) and (60a), defining the wave function inside the well, can now be solved, so that the entire wave function can be expressed in terms of the single constant  $D$ , defined in eq. (58). The constant  $D$  can be evaluated by normalizing the wave function.

**Problem 9:** Show by obtaining the wave function that the number of nodes is equal to  $N$ .

**13. Application of Expansion Theorem.** In Chap. 10, Sec. 22, it was pointed out that an arbitrary function can be expanded as a series of eigenfunctions of any Hermitian operator. Let us now apply this theorem to the Hamiltonian operator for the square well potential. The eigenfunctions must include the continuous spectrum of eigenvalues appearing when  $E > 0$  and also all bound states with  $E < 0$ .

At first sight, it may not be clear why the bound states are needed. The reason is that within the well the eigenfunctions for  $E > 0$  are so distorted by the potential that they are unable to express certain types of functions at all. The functions which cannot be expressed as an

integral of continuum eigenfunctions are, in fact, just the bound-state wave functions. To see this in greater detail, let us note that the bound-state eigenfunctions are orthogonal to the continuum functions (see Chap. 10, Sec. 24). It is, therefore, impossible to expand the bound-state functions in terms of the continuum functions for, according to Chap. 10, eq. (55) the expansion coefficient is just

$$C_x = \int \psi_x^*(x) \psi_B(x) dx$$

which is zero when  $\psi_x$  is a bound-state wave function, and  $\psi_x$  belongs to the continuum. Thus, to express all possible functions, we must sum over bound states, as well as integrate over the continuous spectrum.

14. **Application to Deuteron.** So far, we have considered only a one-dimensional problem, whereas all actual problems are three-dimensional. But we shall see in Chap. 15 that in terms of the radius  $r$ , the wave equation for  $\psi$  is similar to the one-dimensional wave equation that we have given here. In fact, for the special case that  $\psi$  is a function of  $r$  only, and not of the spherical polar angles  $\vartheta$  and  $\varphi$ , the equations will be shown to be identical with the one-dimensional case.† There is, however, one important new restriction, namely, that the wave function must always be zero at the origin. This arises, as we shall see, from the requirement that certain functions remain finite as  $r \rightarrow 0$ . For the present, let us merely accept this requirement.

To find out which bound-state wave functions satisfy the requirement that  $\psi = 0$  at  $x = 0$ , we refer to eq. 57, which gives the value of  $\psi$  within the potential well. At  $x = 0$ , we have

$$\psi = B + C = 0$$

The additional requirement is, therefore, that  $B = -C$ . From eq. (57) this is seen to be the equivalent of

$$\left(1 + \frac{ip_1}{p_2}\right) \exp\left(\frac{-iap_2}{\hbar}\right) = -\left(1 - \frac{ip_1}{p_2}\right) \exp\left(\frac{iap_2}{\hbar}\right)$$

Writing  $p_1/p_2 = \tan \varphi$ , we obtain

$$\exp\left[-i\left(\frac{ap_2}{\hbar} - \varphi\right)\right] = -\exp\left[i\left(\frac{ap_2}{\hbar} - \varphi\right)\right]$$

or

$$\cos\left(\frac{ap_2}{\hbar} - \varphi\right) = 0$$

Hence

$$\varphi = \frac{ap_2}{\hbar} + \frac{N\pi}{2}$$

where  $N$  is an odd integer. Comparing this with eq. (52), we see that if  $N$  is restricted to odd values in eq. (52), then the two equations are

† See Chap. 15, Sec. 3.

equivalent. We therefore conclude that all bound solutions of the three-dimensional problem must have  $N$  odd. As shown in Sec. 10, no such bound solution is possible unless  $V_0 \geq \frac{1}{2m} \left(\frac{\hbar}{a}\right)^2 \left(\frac{\pi}{2}\right)^2$  and, in general, a bound solution with a given value of  $N$  is possible only when  $V_0 \geq \left(\frac{\hbar}{a}\right)^2 \left(\frac{1}{2m}\right) \left(\frac{N\pi}{2}\right)^2$ . The number of bound states depends, therefore, on the depth of the potential well, its radius, and the mass of the particle.

The deuteron consists of a neutron and a proton bound together by a force that can be represented by a square well potential (see Sec. 3). Experimentally it has been found that the binding energy\* is 2.237 mev. Using the radius given in Sec. 3,  $r = 2.8 \times 10^{-13}$  cm, we can calculate the depth  $V_0$  necessary to yield this binding energy. It is known that no levels exist below this level.† That is, there is only one bound state. In eq. (63), we therefore set  $N = 1$ . This gives

$$\sqrt{\frac{|E|}{V_0 - |E|}} = -\cot \sqrt{2m(V_0 - |E|)} \frac{a}{\hbar}$$

$$\tan \sqrt{2m(V_0 - |E|)} \frac{a}{\hbar} = -\sqrt{\frac{V_0 - |E|}{|E|}} \quad (66)$$

Let us write

$$\sqrt{2m(V_0 - |E|)} \frac{a}{\hbar} = \xi$$

We obtain

$$\tan \xi = -\frac{\xi}{a \sqrt{2m|E|}} \quad (67)$$

Since  $|E|$ ,  $m$ , and  $a$  are known, we can solve for  $\xi$  graphically and use this result to solve for  $V_0$ . The result is  $V_0 = 21.2$  mev. Note that we must use the reduced mass  $m = M/2$ , where  $M$  is the proton mass, which is also practically equal to the neutron mass. This is because the wave equation really refers to the relative co-ordinates of the neutron and proton. We shall discuss this point in greater detail in connection with the hydrogen atom. (See Chap. 15, Sec. 5.)

**Problem 10:** Obtain  $V_0$  in the manner suggested in the preceding section.

Note that eq. (66) really determines the product  $\sqrt{V_0 - |E|} a$ , and, therefore, also  $(V_0 - |E|)a^2$ . Since  $|E|/V_0$  is small, the knowledge of the deuteron binding energy enables us to determine the approximate product of  $V_0 a^2$ .

\* The binding energy of a bound state is that energy needed to raise the energy to  $E = 0$ , at which point the particles are no longer bound together. It is clear that the binding energy is equal to  $|E|$  in eq. (64).

† H. Bethe, *Elementary Nuclear Theory*, Chap. 7.

The energy for protons would have to be greater than

$$E = \frac{p^2}{2m} \cong 100 \text{ mev}$$

Most experiments in nuclear physics involve much smaller energies ( $\sim 1$  to 20 mev). Furthermore, at energies of 100 mev and higher, there is evidence that the idea whereby the system can be described by a wave equation involving some definite potential function is breaking down. In other words, at very high energies it is likely that quantum theory may have to be seriously modified. As a result, in the nuclear domain, the entire formulation of the theory in terms of a Hamiltonian operator is a tentative procedure, which can be justified only to the extent that it is successful. It must be emphasized, however, that in the domain of atomic physics, which involves distances not shorter than  $10^{-12}$  cm, the concepts of ordinary quantum theory are known by experiment to be on a very solid foundation. Even here, however, it is often necessary to correct the Hamiltonian operator by small terms such as those involving the spin,\* which are not contained in the classical Hamiltonian function.

The net result of this situation is that in certain problems, especially in nuclear physics, it is necessary to guess the potential function and try to verify our guesses by seeing whether they predict results agreeing with experiment. One of the most important types of results is the energy levels of the system in question: for example, in the case of the deuteron, we saw that because there was only one energy level with a depth of 2.237 mev, we could solve for the product of the depth of the potential  $V_0$  and the square of its range,  $a^2$ . If there had been more energy levels, we should have come to different conclusions about the nature of the potential. We must keep in mind, therefore, the possibility of using the observations of energy levels as a tool to investigate potential functions which we cannot measure directly in a classical fashion. We shall return to this type of consideration many times in the future and we shall also stress the role of the study of scattering as a means of probing into the nature of atomic and nuclear systems.†

**17. Wave Packets Made up from Eigenfunctions in the Continuum.** Thus far, in discussing the continuum eigenfunctions ( $E > 0$ ) for the square well potential, we used plane-wave solutions, which spread over all space. Such solutions actually represent an abstraction never realized in practice, because all real waves are bounded in one way or another. A wave packet more closely represents what happens in a real experiment.

For example, we start out with an incident packet, far from the well. This packet moves toward the well, spreading slowly as it moves. When

\* See Chap. 17.

† See Chap. 21, Sec. 11.

**15. Interpretation of Energy Levels in Terms of Uncertainty Principle.** The fact that no bound states are possible unless

$$V_0 > \frac{1}{2m} \left( \frac{h}{a} \right)^2 \left( \frac{\pi}{2} \right)^2$$

is easily understood in terms of the uncertainty principle. To have a bound state, a particle must be localized roughly within the radius of the well. To have a wave function large only in a region of the size of the well, there must also be a range of momenta  $\sim \frac{h}{a}$  and, therefore, energies  $\sim \frac{1}{2m} \left( \frac{h}{a} \right)^2$ .\* Before a particle can be trapped within the well, the potential energy given up when the particle enters the well must be greater than the kinetic energy that the particle obtains merely because it is localized within the radius  $a$ . Thus, no bound states at all are possible unless  $V_0 > \frac{1}{2m} \left( \frac{h}{a} \right)^2$ . If  $V_0$  is barely great enough to provide the kinetic energy necessary to localize the particle within the well, then the binding energy  $|E|$  will be very small. If  $V_0$  is increased, the binding energy becomes greater, and eventually  $V_0$  becomes so great that it can supply the kinetic energy necessary to make the wave function oscillate once within the well. At this point, a new bound state becomes possible. If  $V_0$  is made greater still, eventually a third oscillation becomes possible, then a fourth, etc. Thus, the number of bound states depends on how much deeper the well is than the minimum amount needed to contain the particle within the well.

**16. Use of Observed Energy Levels to Provide Information about the Potential.** In atomic theory, the usual procedure in quantizing is to start with the classical Hamiltonian function and to form the Hamiltonian operator by replacing the number  $p$ , wherever it occurs, by the operator,  $\frac{h}{i} \frac{\partial}{\partial x}$ . But in many cases, we do not know the classical Hamiltonian function, because our only experience with the system has been on a purely quantum-mechanical level. This is especially true in nuclear physics, since nuclear forces have a very short range. In order for nuclear forces to act in a classical fashion, it would be necessary to have particles for which the de Broglie wavelength  $\lambda = h/p$  was much less than the range of the forces, which is about  $2.8 \times 10^{-13}$  cm. We should, therefore, need momenta much greater than

$$p \cong \frac{h}{2.8 \times 10^{-13}} = \frac{6.6 \times 10^{-27}}{2.8 \times 10^{-13}} = 2.4 \times 10^{-14}$$

\* See Chap. 5, Sec. 5, where a similar discussion is given in connection with the lowest bound state of a hydrogen atom.

it strikes the well, part of it is reflected, and part enters the well.\* The part inside the well reflects back and forth, and part of it goes out to form a transmitted wave, while part returns to contribute to the reflected wave. The reflected wave from inside the well interferes with the wave reflected directly from the well. When the phase relations are right, the reflected wave is canceled by interference of these two parts so that only a transmitted wave is present, and there is a transmission resonance, as described after eq. (50). In general, however, both reflected and transmitted waves are present. If we start with an incident wave packet, the reflected and transmitted waves will also take the form of packets. In this manner, the progress of the wave through the potential can be described as a function of the time. After a long time, no part of the wave will remain inside the potential well.

It is instructive to carry out in detail the solution of the wave equation corresponding to the boundary condition of an incident wave packet as  $t \rightarrow -\infty$ . Let us start with the solution in the region  $x < -a$  (see Fig. 12).

We have for the time-dependent solution

$$\psi(p_1) = \left[ D(p_1) \exp\left(\frac{ip_1 x}{\hbar}\right) + F(p_1) \exp\left(-\frac{ip_1 x}{\hbar}\right) \right] \exp\left[-\frac{iE(p_1)t}{\hbar}\right] \quad (68)$$

where  $D$  and  $F^\dagger$  are, in general, functions of  $p_1$ , and  $E(p_1) = p_1^2/2m$ . To form a packet, it is necessary to integrate  $\psi$  over  $p_1$  with a weighting factor  $f(p_1 - p_0)$ , peaked near some value, which we denote as  $p_0$ . We obtain

$$\psi(x, t) = \int dp_1 f(p_1 - p_0) \exp\left[-\frac{iE(p_1)t}{\hbar}\right] \left[ D(p_1) \exp\left(\frac{ip_1 x}{\hbar}\right) + F(p_1) \exp\left(-\frac{ip_1 x}{\hbar}\right) \right] \quad (69)$$

In general,  $D$  and  $F$  are fairly smooth functions of  $p_1$ , defined by eqs. (47) and (48). For convenience, we can choose  $A$  such that  $D(p_1) = 1$ . This choice yields

$$\frac{A}{4} = \exp\left(-\frac{2ip_2 a}{\hbar}\right) \left[ \left(1 + \frac{p_2}{p_1}\right) \left(1 + \frac{p_1}{p_2}\right) \exp\left(-\frac{2ip_2 a}{\hbar}\right) + \left(1 - \frac{p_2}{p_1}\right) \left(1 - \frac{p_1}{p_2}\right) \exp\left(\frac{2ip_2 a}{\hbar}\right) \right]^{-1} \quad (70)$$

\* In any given instance, the electron is either reflected or transmitted, but the intensities of the respective waves yield the probabilities that each of these processes takes place.

† We are using  $F$  here instead of  $E$ , which was used in the same place in eq. (42).

and, after rearranging,

$$F = -i(p_1^2 - p_2^2) \exp\left(-\frac{2ip_2 a}{\hbar}\right) \sin\left(\frac{2p_2 a}{\hbar}\right) \left[ 2p_1 p_2 \cos\left(\frac{2p_2 a}{\hbar}\right) + i(p_1^2 + p_2^2) \sin\left(\frac{2p_2 a}{\hbar}\right) \right] / \left[ 4p_1 p_2^2 + (p_1^2 - p_2^2) \sin^2\left(\frac{2p_2 a}{\hbar}\right) \right] \quad (71)$$

It is often convenient to write

$$F(p_1) = R(p_1) e^{-i\varphi_1} \quad (72)$$

where  $R(p_1) = |f(p_1)|$ .

(Note that  $p_2$  is expressed in terms of  $p_1$ .) We obtain

$$\varphi_1 = \frac{2p_1 p_2 a}{\hbar} + \tan^{-1} \left( \frac{2p_1 p_2}{p_1^2 + p_2^2} \cot \frac{2p_2 a}{\hbar} \right) \quad (73)$$

Insertion of these values into eq. (69) for  $\psi$  now yields

$$\psi(x, t) = \int dp_1 f(p_1 - p_0) \exp\left(-\frac{iE(p_1)t}{\hbar}\right) \left\{ \exp\left(\frac{ip_1 x}{\hbar}\right) + R(p_1) \exp\left[-i\left(\frac{p_1 x}{\hbar} + \varphi_1(p_1)\right)\right] \right\} \quad (74)$$

To find the place where  $\psi$  is a maximum, we look for the place where the phase of the wave has an extremum when differentiated with respect to  $p_1$ . This insures that many waves of different  $p_1$  will add up in phase, thus producing a peak (see Chap. 3, Sec. 2).

For an incident wave, the phase has an extremum when

$$\left. \begin{aligned} \frac{\partial}{\partial p_1} \left( \frac{x}{\hbar} p_1 - E(p_1) \frac{t}{\hbar} \right)_{p_1=p_0} &= 0 \\ x = \left( \frac{\partial E}{\partial p_1} \right)_{p_1=p_0} t &= \frac{p_0}{m} t \end{aligned} \right\} \quad (75)$$

or when

As  $t \rightarrow -\infty$  we see that this point recedes indefinitely to the left. But as  $t \rightarrow +\infty$ , this point would have to be at  $x \rightarrow +\infty$ . Since the incident wave function has meaning only for  $x$  negative, it is clear that after  $t = 0$ , the incident wave disappears altogether, as it should.

Let us now look at the reflected wave. The condition for an extremum of its phase is

$$\left. \begin{aligned} \frac{\partial}{\partial p_1} \left( \frac{x}{\hbar} p_1 + \varphi_1(p_1) + E(p_1) \frac{t}{\hbar} \right)_{p_1=p_0} &= 0 \\ x = -\left( \frac{\partial E}{\partial p_1} \right)_{p_1=p_0} t - \hbar \left( \frac{\partial \varphi_1}{\partial p_1} \right)_{p_1=p_0} &= -\frac{p_0}{m} t - \hbar \left( \frac{\partial \varphi_1}{\partial p_1} \right)_{p_1=p_0} \\ &= -v_0 t - \hbar \left( \frac{\partial \varphi_1}{\partial p_1} \right)_{p_1=p_0} \end{aligned} \right\} \quad (76)$$



Hence

$$\frac{\partial p_2}{\partial p_1} = p_1 \quad \text{or} \quad \frac{\partial p_2}{\partial p_1} = \frac{p_1}{p_2}$$

From eq. (79), we then obtain

$$\begin{aligned} \hbar \frac{\partial \varphi_2}{\partial p_1} = & -2a \frac{p_1}{p_2} \\ & + \frac{\hbar \left[ \left( \frac{2}{p_2} - \frac{p_2}{p_1^2} - \frac{p_1^2}{p_2^3} \right) \tan 2p_2 \frac{a}{\hbar} + \frac{2a}{\hbar} \left[ \left( \frac{p_1}{p_2} \right)^2 + 1 \right] \sec^2 \left( 2p_2 \frac{a}{\hbar} \right) \right]}{1 + \frac{1}{4} \left( \frac{p_1}{p_2} + \frac{p_2}{p_1} \right)^2 \tan^2 \left( 2p_2 \frac{a}{\hbar} \right)} \end{aligned} \quad (83)$$

It is readily verified that when  $p_1 = p_2 = p_0$  (no barrier),  $\Delta t = 0$ . If  $p_1 \neq p_2$ , the result is rather complex, because there are two effects operating in opposite directions. First, the particle is speeded up as it enters the well; this should tend to make  $\Delta t$  negative. Second, the particle is reflected back and forth inside the well. This should tend to make  $\Delta t$  positive. Near a transmission resonance, the latter effect will win out, particularly if  $p_1 \ll p_2$ , because the reflection coefficient is then very high. Let us now calculate  $\Delta t$ . We note that at a transmission resonance

$$\tan \frac{2p_2 a}{\hbar} = 0 \quad \text{and} \quad \sec^2 \frac{2p_2 a}{\hbar} = 1$$

We get

$$v_0 \Delta t = -\frac{2ap_1}{p_2} + a \left[ 1 + \left( \frac{p_1}{p_2} \right)^2 \right] \quad (84)$$

We note when  $p_1/p_2$  is small,  $\Delta t$  is positive and approximately equal to  $a/v_0$ , where  $v_0$  is the velocity of the particle *outside* the well. Since the particle actually goes faster inside the well in the ratio of  $p_2/p_1$ , it must suffer a number of reflections of the order of  $p_2/p_1$ . According to eq. (11), this is proportional to the inverse of the transmission coefficient; hence the delay is seen to be caused solely by the process of reflection.

**Problem 11:** Find the time delay for the reflected wave at a transmission resonance and interpret the result in terms of reflection of the wave inside the well.

**20. Metastable (or Virtual) States of Trapping an Object within a Well.** The previous discussion indicates that even when an object has enough energy to escape, it may, after entering the well, be reflected back and forth many times before it manages to get back out. This will happen if  $p_1 \ll p_2$ , i.e., if the depth of the well is much greater than the kinetic energy of the particle outside the well, and if the conditions are such that there is a transmission resonance ( $2p_2 a/\hbar = N\pi$ ). (From eq. 84, one can easily show that if we are not near such a resonance, the time delay is not very great, so that there is little likelihood of trapping the particle.) If the number of reflections of the wave is very great, the

As  $t \rightarrow +\infty$ , we see that  $x \rightarrow -\infty$ . Hence, a reflected wave packet appears after the incident wave packet has struck the well. The significance of the term involving  $\partial \phi_1/\partial p_1$  will be discussed in Sec. 19.

**18. Wave Packet for Transmitted Wave.** The transmitted wave amplitude is

$$\psi(x, t) = \int dp_1 f(p_1 - p_0) \exp \left[ -\frac{iE(p_1)t}{\hbar} \right] A(p_1) \exp \left( \frac{ip_1 x}{\hbar} \right) \quad (77)$$

As in eq. (72) we write

$$A = |A| e^{i\varphi_1}$$

But, according to eq. (70),

$$A = \frac{\exp(-2ip_2 a/\hbar) \cos(2p_2 a/\hbar) + i/2(p_1/p_2 + p_2/p_1) \sin(2p_2 a/\hbar)}{\cos^2(2p_2 a/\hbar) + \frac{1}{4}(p_1/p_2 + p_2/p_1)^2 \sin^2(2p_2 a/\hbar)} \quad (78)$$

The phase  $\varphi_2$  can then be written

$$\varphi_2 = -\frac{2p_2 a}{\hbar} + \tan^{-1} \left[ \frac{1}{2} \left( \frac{p_1}{p_2} + \frac{p_2}{p_1} \right) \tan 2p_2 \frac{a}{\hbar} \right] \quad (79)$$

The wave function becomes

$$\psi(x, t) = \int dp_1 f(p_1 - p_0) |A| \exp \left\{ i \left[ p_1 \frac{x}{\hbar} + \varphi_2 - E(p_1) \frac{t}{\hbar} \right] \right\} \quad (80)$$

The maximum of the wave packet occurs where the derivative of the argument of the exponential is zero, or where

$$x = \left( \frac{\partial E}{\partial p_1} \right)_t \frac{t}{p_1 - p_0} - \hbar \left( \frac{\partial \varphi_2}{\partial p_1} \right)_{p_1 = p_0} = \frac{p_0 t}{m} - \hbar \left( \frac{\partial \varphi_2}{\partial p_1} \right)_{p_1 = p_0} \quad (81)$$

As  $t \rightarrow +\infty$  the maximum appears in the region where  $x > a$ . Thus, after sufficient time, the transmitted wave appears and travels with the group velocity  $v_0 = p_0/m$ .

**19. Time Delay of Wave as It Crosses Potential Well.** If there were no potential well causing the wave to be reflected, we should expect the transmitted wave to move with its center at  $x = p_0 t/m$ . The additional term in eq. (81) represents a time delay, as can be seen by noting that it causes a given value of  $x$  to be reached later than if this term were not present.

Let us now evaluate the time delay of the transmitted wave:

$$\Delta t = \frac{\hbar}{v_0} \left( \frac{\partial \varphi_2}{\partial p_1} \right)_{p_1 = p_0} \quad (82)$$

In differentiating  $\varphi_2$ , we must use the fact that

$$p_1^2 = 2m(E - V_0) = p_1^2 - 2mV_0$$

system appears to be in an almost stationary state, which, however, gradually decays, as the wave is slowly transmitted after many internal reflections. Such a state is called a virtual, or a metastable, level. Its energy is positive, in contrast to that of a true bound state, which is always negative. Its lifetime is given by  $\Delta t$ , as calculated in eq. (84).

Because such a metastable wave function constitutes, in effect, a wave packet which passes through the nucleus in a time  $\Delta t$ , its energy must, according to the uncertainty principle, fluctuate by

$$\Delta E \cong \frac{\hbar}{\Delta t}$$

Another way of obtaining the same result is to note that a metastable state can have physical significance only when the incident wave packet is so narrow that it passes a given point in a time less than the delay occurring inside the well. If this condition is not satisfied, then the time delay will be blotted out by the initial width of the packet itself, and no time delay will be observable. But to form a packet narrower than  $\Delta t$ , we need a range of energies greater than  $\hbar/\Delta t$ . Thus, a metastable state can exist only under conditions in which the energy is left undefined by this amount.

**21. Metastable Singlet State of Deuteron.** An important case of a metastable state, in which a particle is bound temporarily by reflection from a sharp edge, occurs in what is called the *singlet state* of the deuteron. Previously we stated that the neutron attracted the proton with a potential energy of 21.2 mev. Actually this is the potential only when the neutron spin is parallel to the proton spin. If the spins are antiparallel, the potential is less\* and, in fact, equal to 11.85

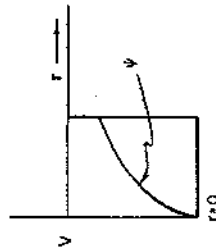


FIG. 18

mev. Remembering that in a three-dimensional problem we must have  $\psi = 0$  at the origin, we can show that this reduction in potential is sufficient to prevent the wave function from curving downward to meet a decaying exponential at the edge of the well, so that if the spins are antiparallel, there are no bound states. In fact, for  $E = 0$ , it turns out that the wave starting out zero at the origin does not quite reach a phase of  $\pi/2$  at the edge of the well. This result is illustrated in Fig. 18. But with a small positive energy ( $\cong 40$  kev), the phase becomes  $\pi/2$  at the edge of the well. According to the discussion following eq. (50), this is the condition for a transmission resonance and, therefore, for a virtual level. As a result, there should be a metastable singlet level at a very low positive energy. The lifetime is

$$\Delta t = \frac{\hbar}{\psi_0} \quad (85)$$

\* H. Bethe, *Elementary Nuclear Physics*, p. 43.

where  $v_0$  is the velocity outside the well. The number of reflections is of the order of  $\frac{v_{(\text{inside})}}{v_0} = \sqrt{\frac{E + V_0}{E}}$ . With  $V_0 = 20$  mev and  $E \cong 40$  kev, this number is of the order of 20.

We shall see in Chap. 12, Sec. 18, that much longer-lived metastable states are possible, as a result of reflection of a particle from a potential barrier. In fact, metastable states are extremely common in nuclear physics and are one of the most important nuclear phenomena now being studied.