CHAPTER IV.

THE GENERAL METHOD FOR SOLVING SCHRÖDINGER'S EQUATION ON AN ANALOGUE COMPUTER.

The earlier chapter of this thesis emphasized the use of the basic computing elements of an analogue computer. An integrated review of the steps necessary to solve the Schrödinger equation for analogue computation will now be discussed.

(4.1) Problem Analysis.

A mathematical description of Schrödinger's equation was given in the last chapter and we stated Schrödinger's equation in the form

$$\frac{d^2\psi(x)}{dx^2} + \frac{2m}{\hbar^2}\left[E-V(x)\right]\psi(x) = 0. \quad \text{------ (4.1)}$$

Since the computer independent variable is time, denoted by t, we must to change the independent variable x of equation (4.1) to the time variable. The relationship between the physical Schrödinger equation and it's computer representation are shown in table 1.

Physical Schrödinger Equation	Computer Representation
Variable x $\psi(x)$ $\frac{d^2\psi(x)}{dx^2} + \frac{2m}{\hbar^2}\left[E-V(x)\right]\psi(x) = 0$	Variable t $\psi(t)$ $\frac{d^2\psi(t)}{dt^2}+\frac{2m}{\hbar^2}\left[E-V(t)\right]\psi(t)=0$ ------ (4.2)

(4.2) Rearranging the Equation.

Schrödinger's equation (4.2) is rearranged to have only the second derivative on the left-hand side.

$$\frac{d^2\psi(t)}{dt^2} = -\frac{2mE}{\hbar^2}\psi(t) + \frac{2m}{\hbar^2}V(t)\,\psi(t) \text{ ----- } (4.3)$$

Successive integration of the second derivative will yield $\frac{d\psi(t)}{dt}$ and $\psi(t)$. For solution on the computer it is assumed that $\frac{d^2\psi(t)}{dt^2}$ exists as the input to an integrator. After producing $\psi(t)$ by integration one can sum appropriately all terms on the right-hand side of the equation to form $\frac{d^2\psi(t)}{dt^2}$. This sum of terms must therefore be fed into the integrator where $\frac{d^2\psi(t)}{dt^2}$ was assumed to exist. (see later, Fig.4.1)

Let $A = \frac{2mE}{\hbar^2}$,

$B = \frac{2m}{\hbar^2}$,

and represent $\frac{d^2\psi(t)}{dt^2}$ by $\ddot{\psi}(t)$. Equation (4.3) then becomes

$$\ddot{\psi}(t) = -A\psi(t) + BV(t)\,\psi(t). \text{ --------- } (4.4)$$

Equation (4.4) is the mathematical computer equation corresponding to the physical Schrödinger equation whose solutions are to be demonstrated on the analogue computer.

(4.3) Block Diagram.

The block diagram is a preliminary computer diagram ignoring scales, signs, and gains, but showing the main

computing elements and their interconnections. It is frequently useful for obtaining an estimate of the amount of computing equipment needed, and for producing at a later time a neat computer circuit diagram. The block diagram of equation (4.4) is shown in Fig.4.1.

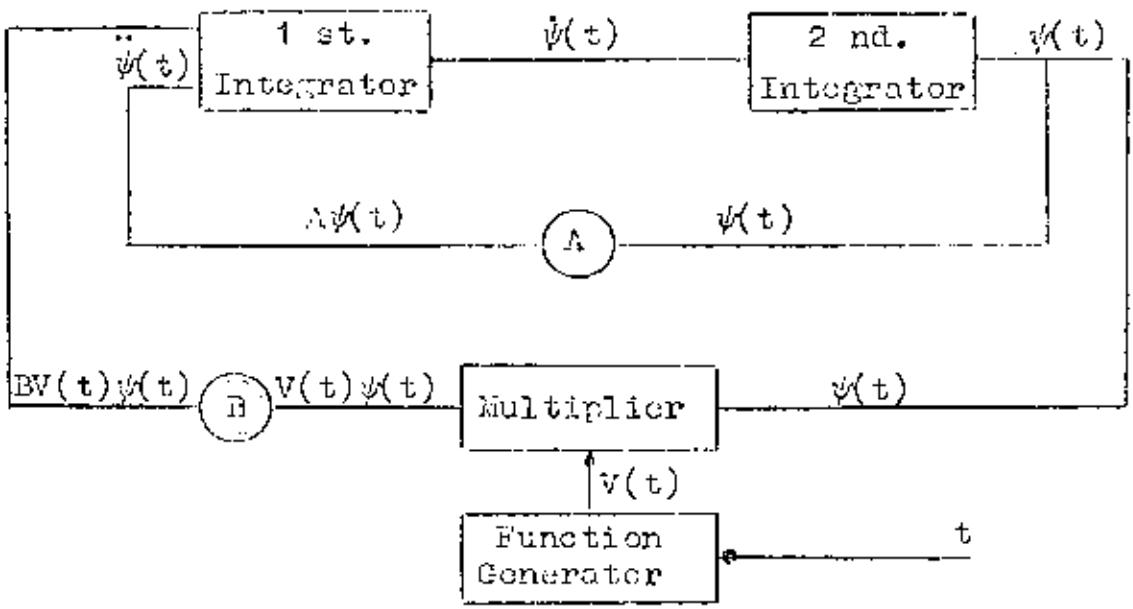


Fig.4.1: The block diagram for equation (4.4).

(4.4) The Scale Factor[12]

Before the Schrödinger equation can be solved on an analogue computer, it is necessary to determine the time of solution desirable, and the output amplitude of the solution. These two factors will now be discussed:

(a) Time-Scale Factor

The minimum time for a computer run is normally determined by the speed of response of the computing and

recording units. When using an oscilloscope for read-out, a short solution time is desirable and for a recorder , a longer solution time is better. The output time desired is determined by the RC constant of the integrating amplifiers.

(b) Amplitude-Scale Factor

When we are preparing the Schrödinger equation for solution on an analogue computer, it is necessary to ensure that the voltages representing the variables will never have values larger than the allowable voltage of an analogue computer. The normal operating range of the operational amplifiers in the Heath Analogue Computer is ±100 volts. Maximum output voltages near zero should be avoided. If the output voltage would exceed the allowable voltage of the analogue computer, it must be scaled down. The maximum values of the physical variables must therefore be scaled by the relationship:

$$\frac{\text{Max. allowable voltage}}{\text{Max. value of physical variable}} = \text{Scale factor}$$

and (Max. value of physical variable)$\times a \leq$ Max. allowable voltage,

where $a \leq \frac{100}{\text{Max. value of physical variable}}$, is called the amplitude-scale factor.

For solving equation (4.4), we can select a suitable time-scale by choosing the values of R and C of the

integrating amplifiers. The variables $\psi(t)$ and $\ddot{\psi}(t)$ are amplitude scaled within ±100 volts, the allowable range of the Heath Analogue Computer, and we must make sure that the working voltages of each amplifier in the circuit do not exceed 100 volts. In the case of equation (4.4) the scaling is taken care of in the coefficients A and B.

The computer circuit of equation (4.4) is shown in Fig.4.2.

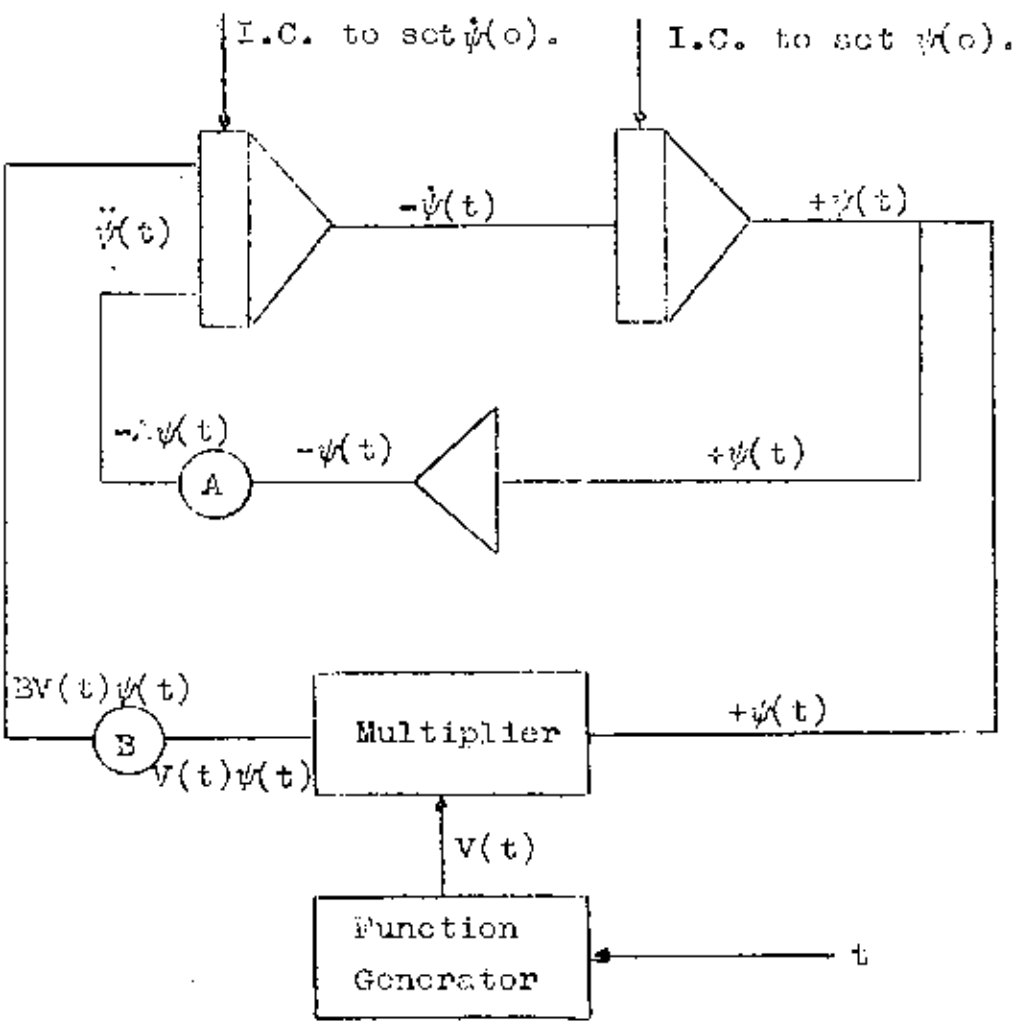


Fig.4.2: Computer Circuit of Equation (4.4).

In solving equation (4.4) on the analogue computer, we will divide our problem into 5 cases as follows:

Case.I: When $V(t) = o$, wave function represents the motion of a free particle with zero potential energy. From equation (4.4) we have

$$\ddot{\psi}(t) = -A\,\psi(t). \qquad \text{---------- (4.5)}$$

The computer circuit of equation (4.5) is a simplified form of the circuit in Fig.(4.2) and is shown in Fig. 4.3.

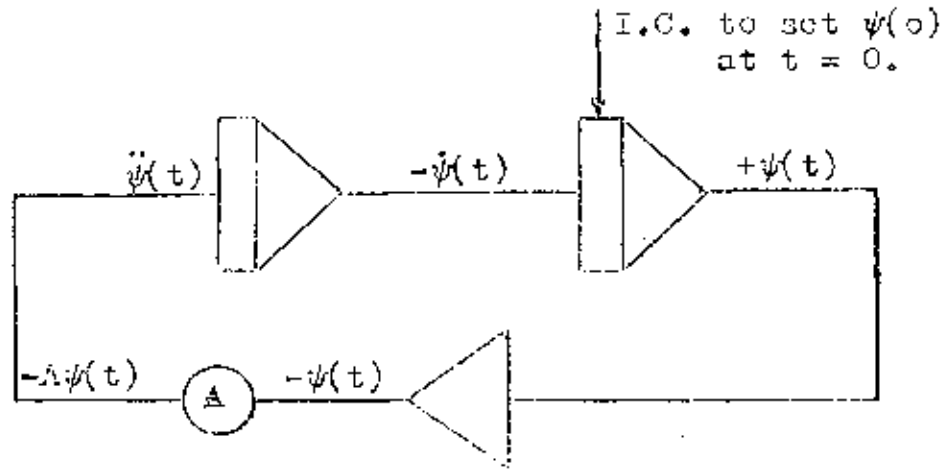


Fig.4.3: Computer Circuit of Equation (4.5).

In the above circuit, if we feed a voltage which is proportional to $A\psi(t)$ and hence $\ddot{\psi}(t)$ into the first integrator, the output of that integrator will be $-\dot{\psi}(t)$. Then the voltage will be $\psi(t)$ at the output of the second integrator. And if we feed $\psi(t)$ through the sign-changer and a potentiometer which multiplies by A, then it will become the input

of the first integrator.

The computer circuit showing the elements of the operational amplifiers for patching is shown in Fig.4.4.

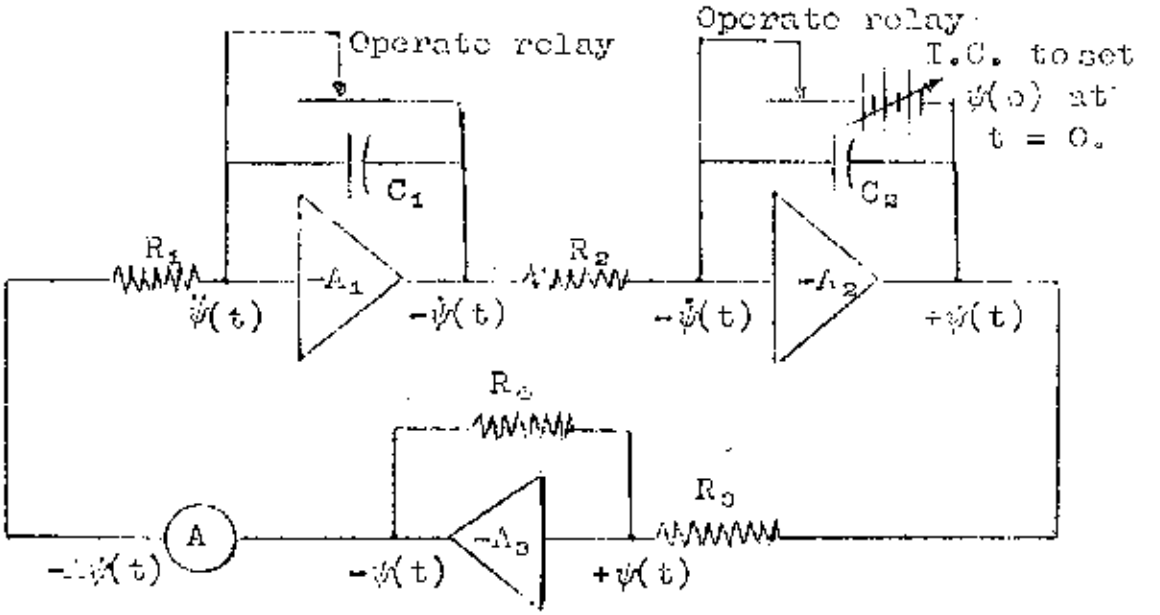


Fig.4.4: Actual Circuit for Patching of Equation (4.5).

In Fig.4.4, we connect the operate relay across the integrating capacitors, because the solution of the problem leaves the integrating capacitors charged, and it is necessary to remove this charge before the problem can be rerun. We connect the initial condition power supply, for the initial condition (I.C.) to set the value $\psi(o)$ at $t = o$, into the second integrator, and assume $\dot{\psi}(o) = o$. The coefficient A is set by a potentiometer.

All the resistors in the computer circuit of Fig.4.4 are 100 KΩ (Kilo-ohm), and both capacitors are 0.01 μf.

(Microfarad). Therefore the RC time constant of the integrators is $(100 \times 10^{3}) \times (0.01 \times 10^{-6}) = 0.001$seconds.

(4.5) Patching

When we have the actual computer circuit as shown in Fig.4.4, the problem is set up on the computer machine by connecting the required components together. This is called patching.

Since we use the oscilloscope for read-out, and the solution time of our problem was chosen for display on a cathode ray oscilloscope, it is convenient to use one of the D.C. amplifier to provide time base of the oscilloscope. This may be done as shown in Fig.4.5.

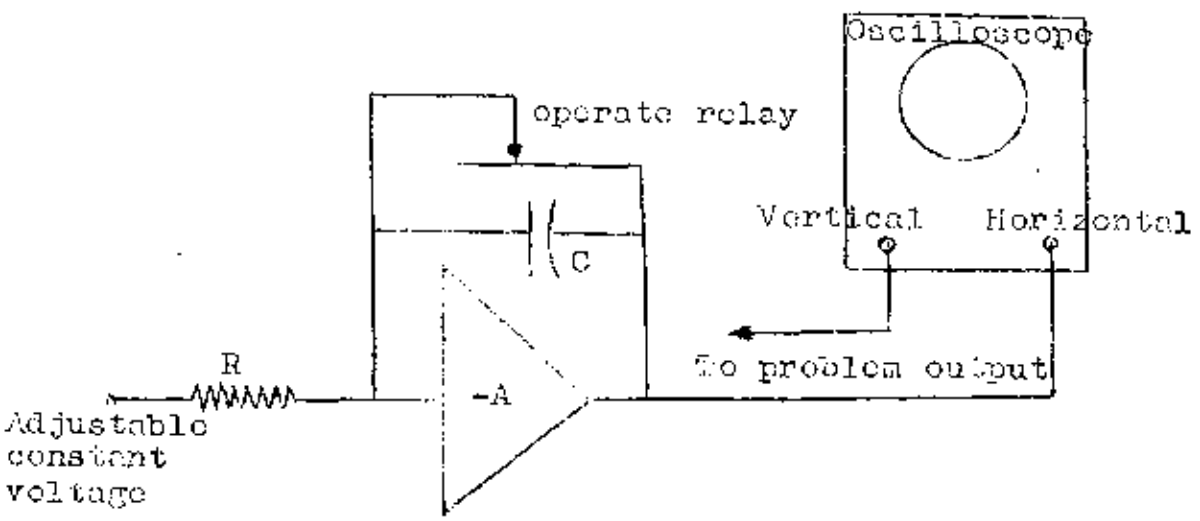


Fig.4.5: Time base circuit

The value of RC is the same as for the integrating amplifiers.

(4.6) Insertion of Problem Parameter

When we have patched the computer circuit, we adjust the coefficient potentiometer A, to set the value of A between 0 and 1, and adjust the initial condition (I.C.), to set $\psi(o)$ between ±100 volts.

(4.7) Solution

For a suitable value of A and $\psi(o)$, we obtain the solution on the oscilloscope as shown in Fig.4.6.

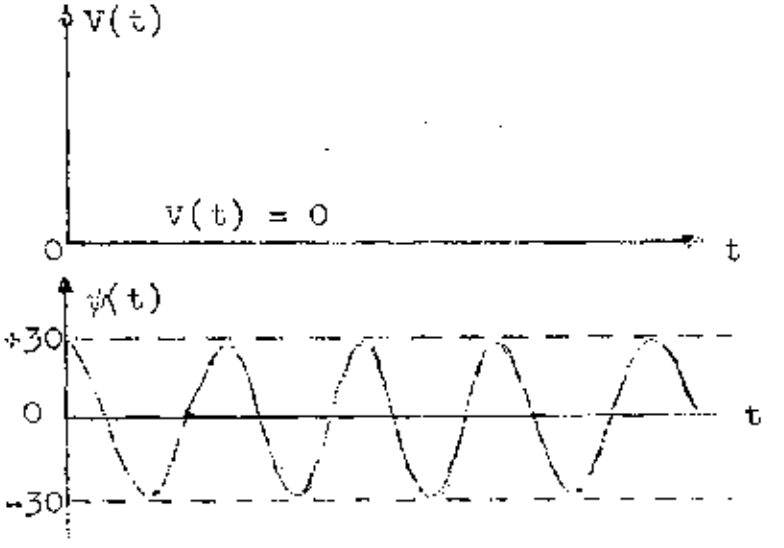


Fig.4.6: The Solution of Equation (4.5) on Oscilloscope.

The well known mathematical solution of equation (4.5) has the form:

$$\psi(t) = D_1 \cos \sqrt{A}\, t + D_2 \sin \sqrt{A}\, t \quad \text{---- (4.6)}$$

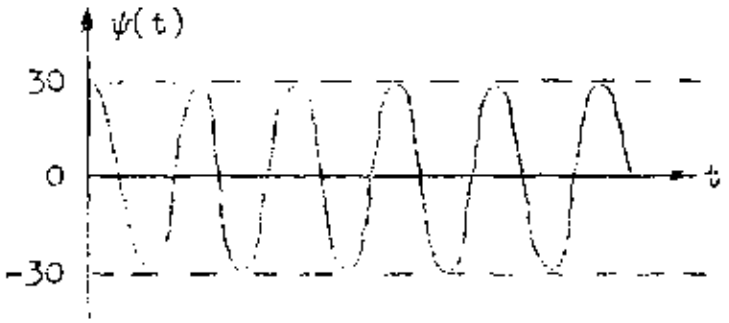
where D_1 and D_2 are arbitrary constants.

For initial condition at t = 0 , $\psi(o) = 30$, $\dot{\psi}(o) = 0$, we have

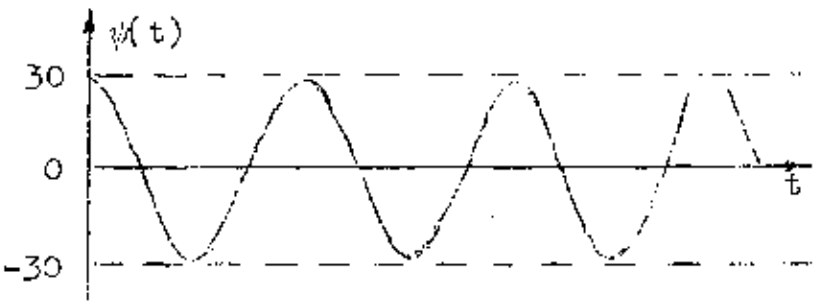
$$\psi(t) = 30 \cos \sqrt{A}\, t. \quad \text{---------- (4.7)}$$

which is the shape obtained on the oscilloscope.

When we adjust the potentiometer A to vary the value of A corresponding to the energy of the particle ($A = \frac{2m}{\hbar^2}E$), the solution on the oscilloscope will be varied also. The effect on the solution when A is varied, is shown in Fig. 4.7.



a) The solution when A is increased



b) The solution when A is decreased.

Fig. 4.7: The Effect on the Solution when A is Varied.

When we increase the value of A, then the value of E is increased also, and the wavelength of the solution is decreased. When A is decreased, the wavelength is increased as shown in Fig.4.7b.

These solutions illustrate the change in the de Broglie wavelength of the particle according to de Broglie's relation:[15]

$$p = \frac{h}{\lambda}$$

where p is the momentum,

h is Planck's constant,

and λ is the de Broglie wavelength.

For a free particle we have

$$E = \frac{p^2}{2m} = \frac{h^2}{2m\lambda^2}$$

$$\therefore \quad \lambda = \sqrt{\frac{h^2}{2mE}} .$$

We have seen that the solutions on the oscilloscope are in agreement with de Broglie's relation.

If we vary the initial condition $\psi(o)$, the amplitude of wavefunction $\psi(t)$ will be varied. But the wavelength is constant and the effect of the solution is shown in Fig.4.8.

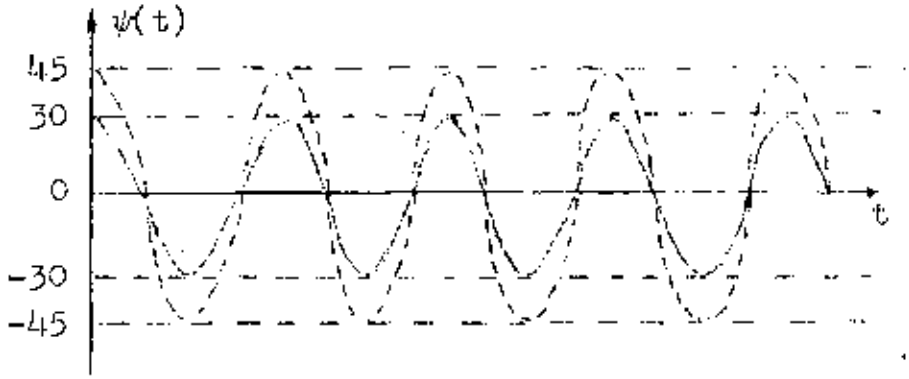


Fig.4.8: The effect of amplitude $\psi(t)$ when $\psi(o)$ varied.

In this example the wavefunction $\psi(t)$ may be used to describe a stream of particles all with energy E./$\psi(t)/^2$ represents the density of particles at each point of the x-axis. The regular fluctuation of the density occurs because the wavefunction obtained by the computer represents two equal streams of particles, one from the left and one from the right, whose waves interfere. The complete solution of equation (4.5) is a complex function, but of course only the real part can be shown on the oscilloscope. By a suitable choice of complex solution a constant value of $/\psi(t)/^2$ may be represented.[14]

[Note: If $\ddot{\psi}(t) = -A\ \psi(t)$, then the solution is

$\psi(t) = A_1\, e^{i\sqrt{A}\,t} + A_2\, e^{-i\sqrt{A}\,t}$; and if $A_1 = 1$, $A_2 = 0$, then $/\psi(t)/^2 = 1$, for all t.]

Case.II. Given $V(t) = V_o$, for all t. The constant potential is shown in Fig.4.9.

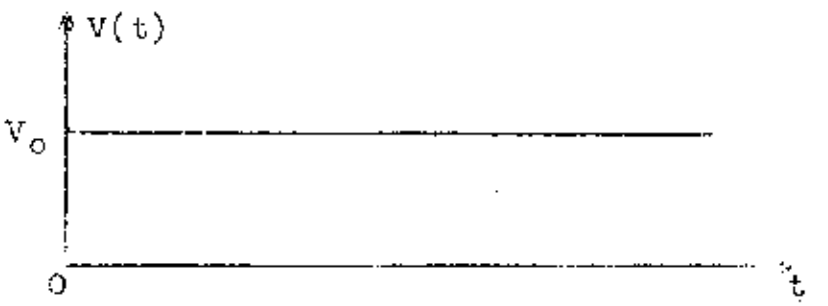


Fig.4.9: The Constant Potential.

The physical interpretation in this case is the motion of particles under a constant potential. From equation (4.4) we have

$$\ddot{\psi}(t) = -A\,\psi(t) + BV_0\psi(t) \quad \text{---------} \quad (4.8)$$

Since V_0 is constant, we let $BV_0 = C$ where C is the arbitrary constant, and we have $C = \frac{2mV_0}{\hbar^2}$, then equation (4.8) becomes

$$\ddot{\psi}(t) = -A\,\psi(t) + C\,\psi(t) \quad \text{----------} \quad (4.9)$$

The procedure used to solve equation (4.9) on an analogue computer is similar to that in case.I. The computer circuit for equation (4.9) is shown in Fig.4.10.

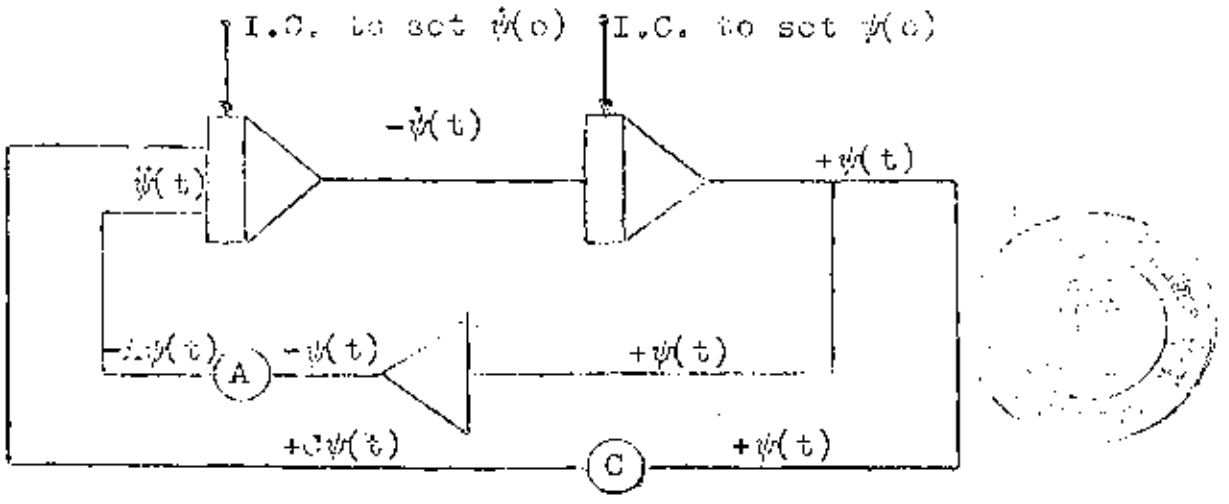


Fig.4.10: The Computer Circuit of Equation (4.9).

In the above circuit, if we adjust C = 0, then the circuit is the same as that in case.I. The actual computer circuit for patching equation (4.9) is shown in Fig.4.11.

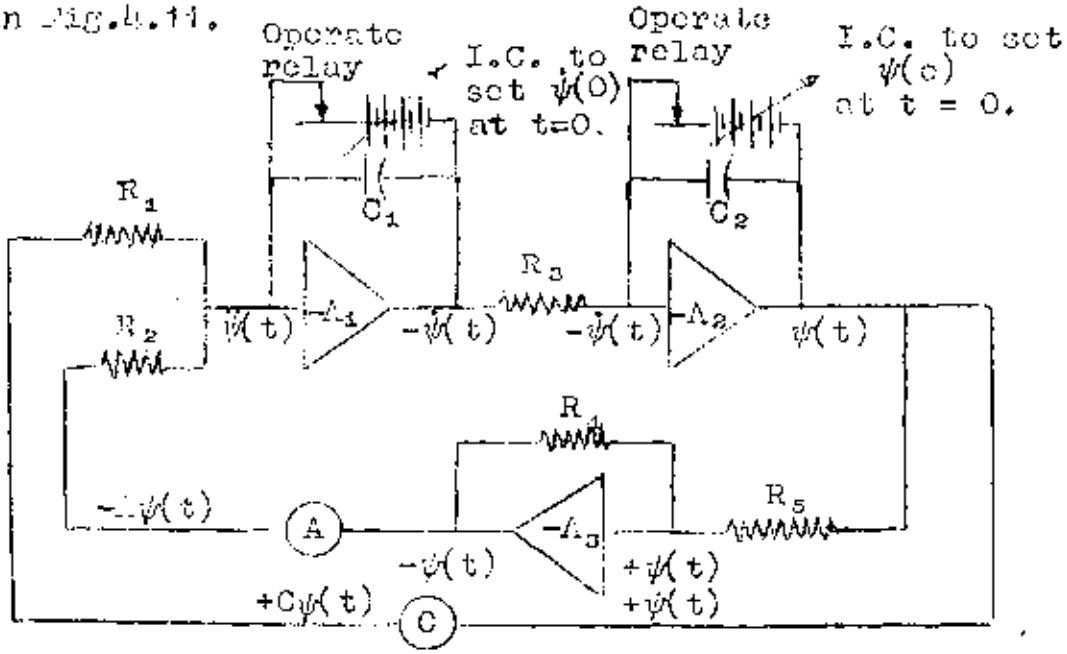


Fig.4.11: The Computer Circuit for Patching of Equation (4.9).

The values of elements R and C are the same as those in the circuit in Fig.4.4. We will consider the method to operate the equation (4.9) in two cases:

Case A: Given $A > C$, since $A = \frac{2mE}{\hbar^2}$ and $C = \frac{2mV_0}{\hbar^2}$, then we have $E > V_0$. We adjust $A \approx 0.6$, $C \approx 0.3$, $\psi = 30$ volts and for the convenience we set $\dot{\psi}(o) = 0$. We obtain the solution on the oscilloscope, as shown in Fig.4.12.

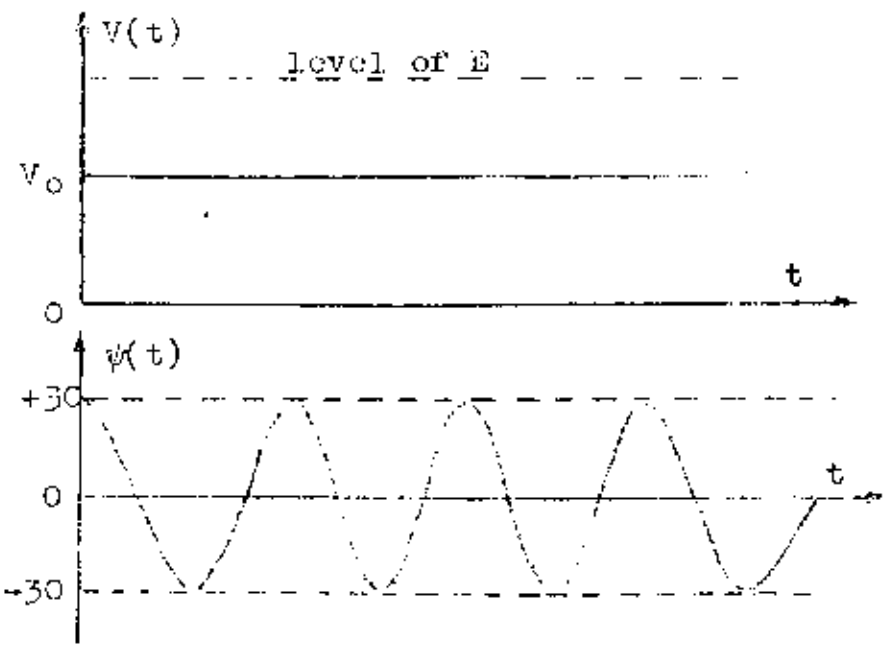


Fig.4.12: The Solution of Equation (4.9) on the Oscilloscope when $A > C$.

The well known mathematical solution of equation (4.9) , when $A > C$ is in the form

$$\psi(t) = A_1 \cos p_1 t + A_2 \sin p_1 t \ , \ p_1 = \sqrt{A-C} \quad \text{---(4.10)}$$

where A_1 and A_2 are arbitrary constants. In this case we have set $\psi(o) = 30$ volts and $\dot{\psi}(o) = 0$ at $t = 0$. The solution in equation (4.10) becomes

$$\psi(t) = 30 \cos p_1 t \qquad \text{---------- (4.11)}$$

The shape of the solution $\psi(t)$ in equation (4.11) is the same as the solution on oscilloscope, as shown in Fig. 4.12. This solution is similar to that for $V(t) = 0$, except that the wavelength is longer for a given value of E. This illustrates the fact that the kinetic energy T is smaller for a given total energy: $T = E - V_o$; if we fix E and increase V_o , then T decreases and the de Broglie wavelength increases.

Case.2: Given $A < C$ and we have $E < V_o$. We set $A \approx 0.3$, $C \approx 0.6$, $\psi(o) = 30$ volts and vary $\dot{\psi}(o)$ between ± 30 volts. We obtain solutions on the oscilloscope as shown in Fig.4.13.

The various solutions shown in Fig.4.13 depends on the value $\dot{\psi}(o)$, because if we adjust $\dot{\psi}(o)$, it is equal to changing the slope of the curve at $t = 0$. First we set $\psi(o)$ to a convenient value (30 volts). Then we adjust $\dot{\psi}(o)$ to make the solution approach $\psi(t) = 0$ at $t \to \infty$ as in curve (2). This solution is described by equation (4.13) below. The other curves (1),(3) occur for the other values of $\dot{\psi}(o)$.

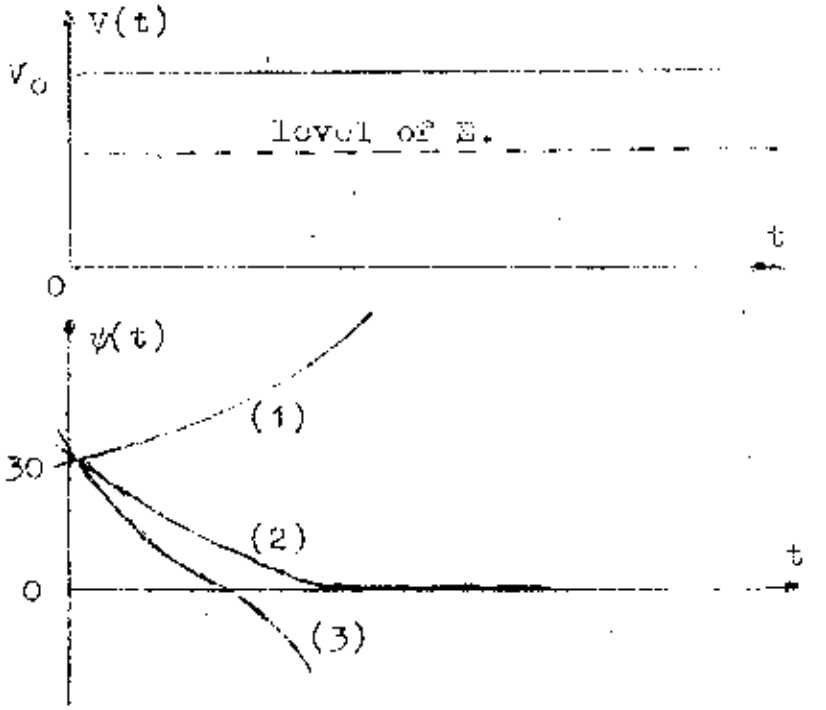


Fig.4.13: Solutions on the Oscilloscope of Equation (4.9) when A < C.

The mathematical solution of equation (4.9) when A < C is in the form

$$\psi(t) = A_3 \exp. p_2 t + A_4 \exp.(-p_2)t \ , \ p_2 = \sqrt{C-A} \quad -- \ (4.12)$$

where A_3 and A_4 are the arbitrary constants.

The solution $\psi(t)$ in equation (4.12) has real exponentials, but we have stated in the last chapter that the wavefunction must be finite. Hence in order that the probability remain finite as $t \to \infty$, it is necessary that we choose $A_3 = 0$. Since $\psi(o) = 30$, at $t = 0$, we have $A_4 = \psi(o) = 30$ volts. Equation (4.12) becomes:

$$\psi(t) = 30 \exp.(-p_2)t \qquad \text{---------- (4.13)}$$

This solution $\psi(t)$ is solution (2) which we obtained on the oscilloscope in Fig.4.13. When A_3 in equation (4.12) is not zero, we obtain solution (1) for $A_3 > 0$ and solution (3) for $A_3 < 0$.

The solutions in Fig.4.13 do not have a physical meaning when $A < 0$ over the whole t-axis, for $\psi(t)$ is then unbounded. Hence a particle is never observed with $E < V_o$ over the whole space. These solutions can only occur in part of the t-axis, such as in the potential step, the potential barrier and the potential well, as discussed later.

Case.III. Potential Step; The potential function V(t) is defined by

$$V(t) = 0 \quad , \quad 0 < t < t_o \ ,$$
$$= V_o \quad , \quad t \geq t_o .$$

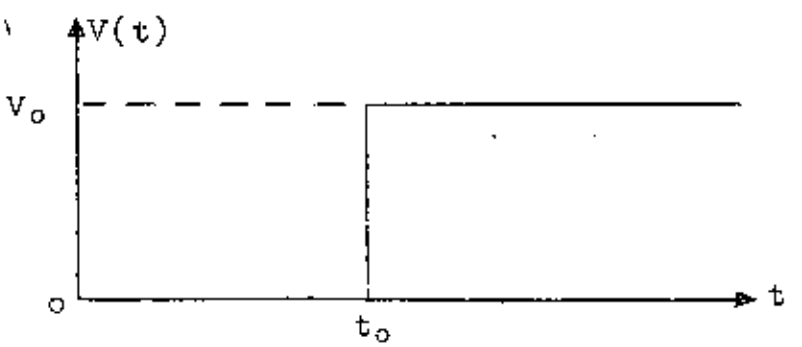


Fig.4.14: The Potential Step

Case.IV. Potential Barrier; The potential function V(t) is defined by

$$V(t) = 0 \quad , \quad t < -t_o \ ,$$
$$= V_o \quad , \quad -t_o \leq t \leq +t_o \ ,$$
$$= 0 \quad , \quad t > -t_o .$$

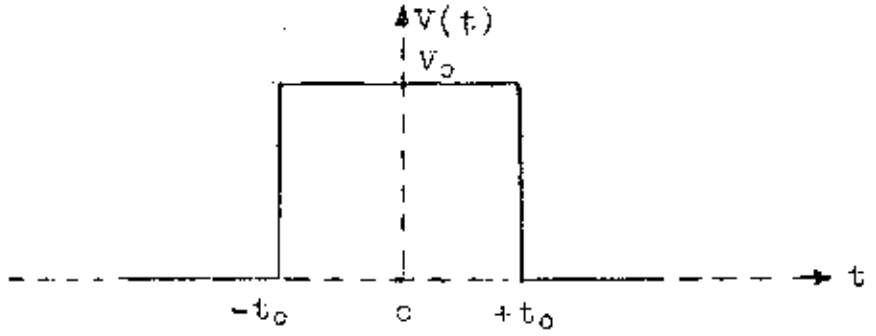


Fig.4.15: The Potential Barrier.

Case.V. Potential Well; The potential function V(t) is defined by

$$V(t) = V_o \quad , \quad t < -t_o \ ,$$
$$= 0 \quad , \quad -t_o \leq t \leq +t_o \ ,$$
$$= V_o \quad , \quad t > +t_o .$$

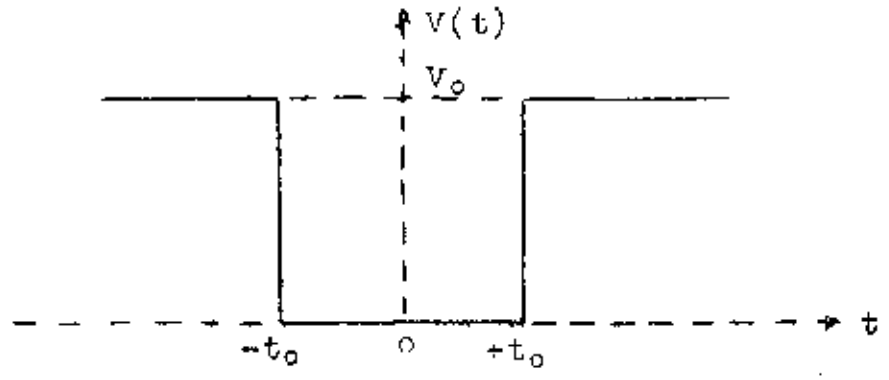


Fig.4.16: The Potential Well.

In cases III, IV, and V the potential function V(t) and the product V(t) ψ(t) varies with t. The mathematical equation has the same form in all three cases and is

$$\ddot{\psi}(t) = -A\psi(t) + BV(t)\psi(t) \text{ -------- } (4.14)$$

The computer circuit for equation (4.14) is shown in Fig.4.17.

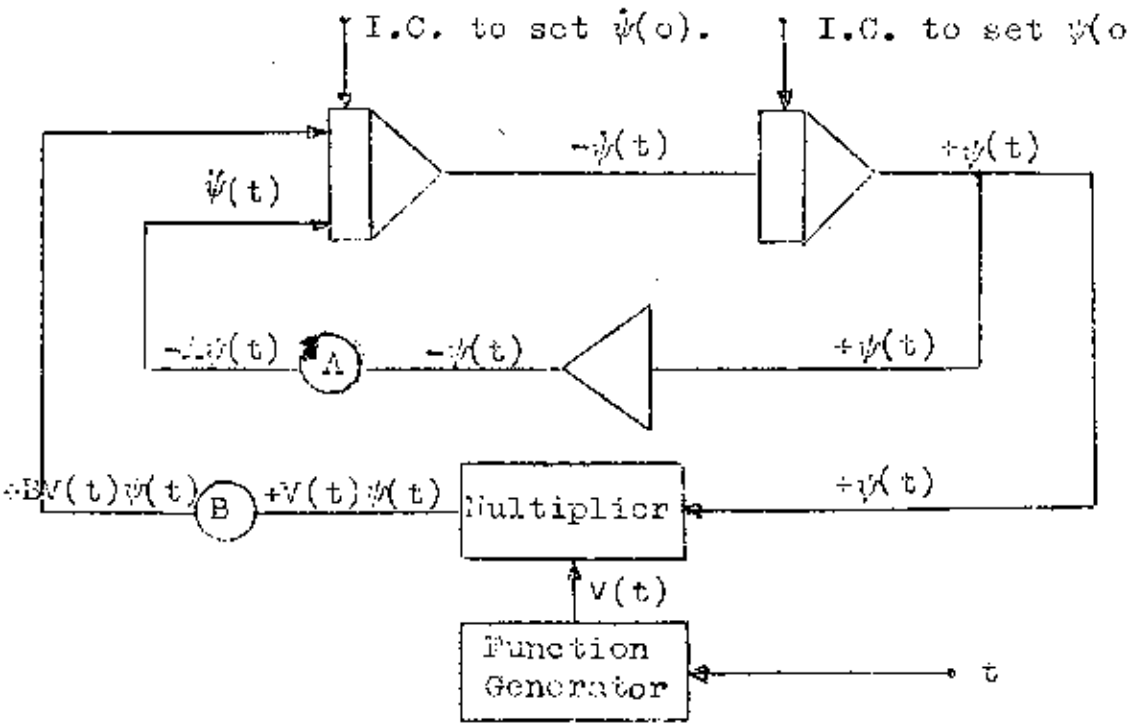


Fig.4.17: The Computer Circuit for Equation (4.14).

In the computer circuit for equation (4.14), we must have a multiplier to multiply the functions V(t) and ψ(t), and a function generator to generate the functions V(t) defined in Fig.4.14, Fig.4.15, and Fig.4.16. The Heath Analogue Computer which I used for my thesis work has no

multiplier or function generator. Hence the concept of the potential step, the potential barrier and the potential well could not be demonstrated on it. But we will discuss techniques for solving equation (4.14) on a complete computer.

The equation and the circuit for quarter-square multiplication are as follows:

$$V(t)\ \psi(t) = \frac{1}{4}\left[\left(V(t)+\psi(t)\right)^2-\left(V(t)-\psi(t)\right)^2\right] \quad \text{---(4.15)}$$

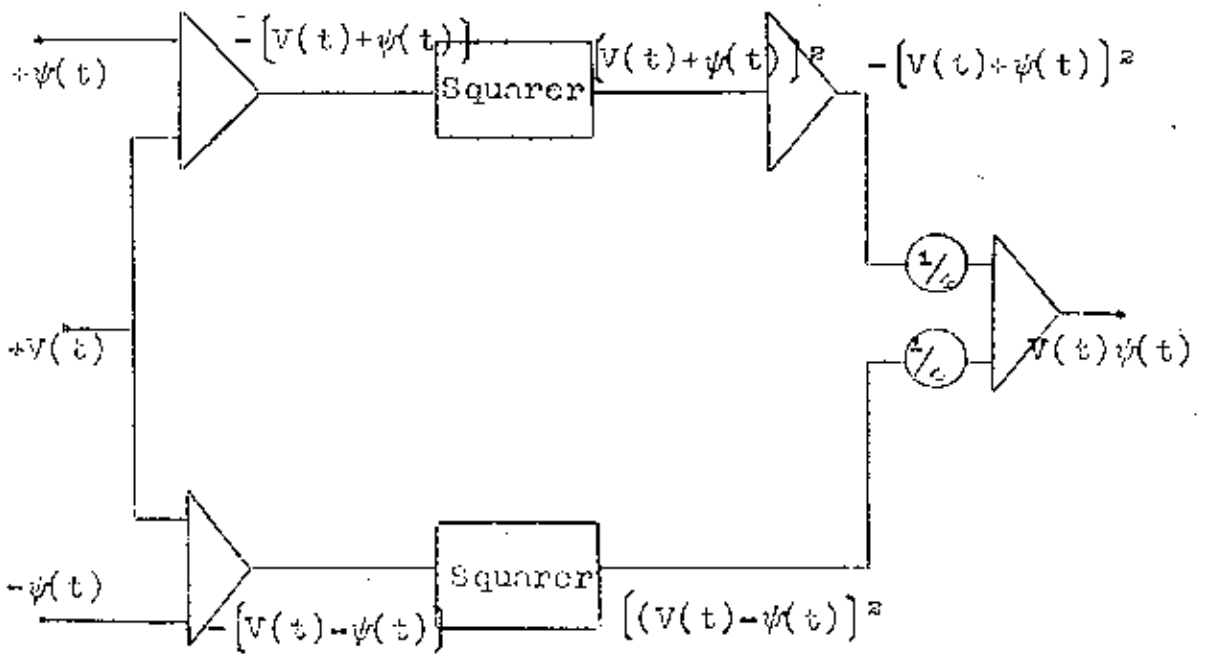


Fig.4.18: The Quarter-Square Multiplier.

The complete computer circuit for equation (4.14) is shown in Fig.4.19.

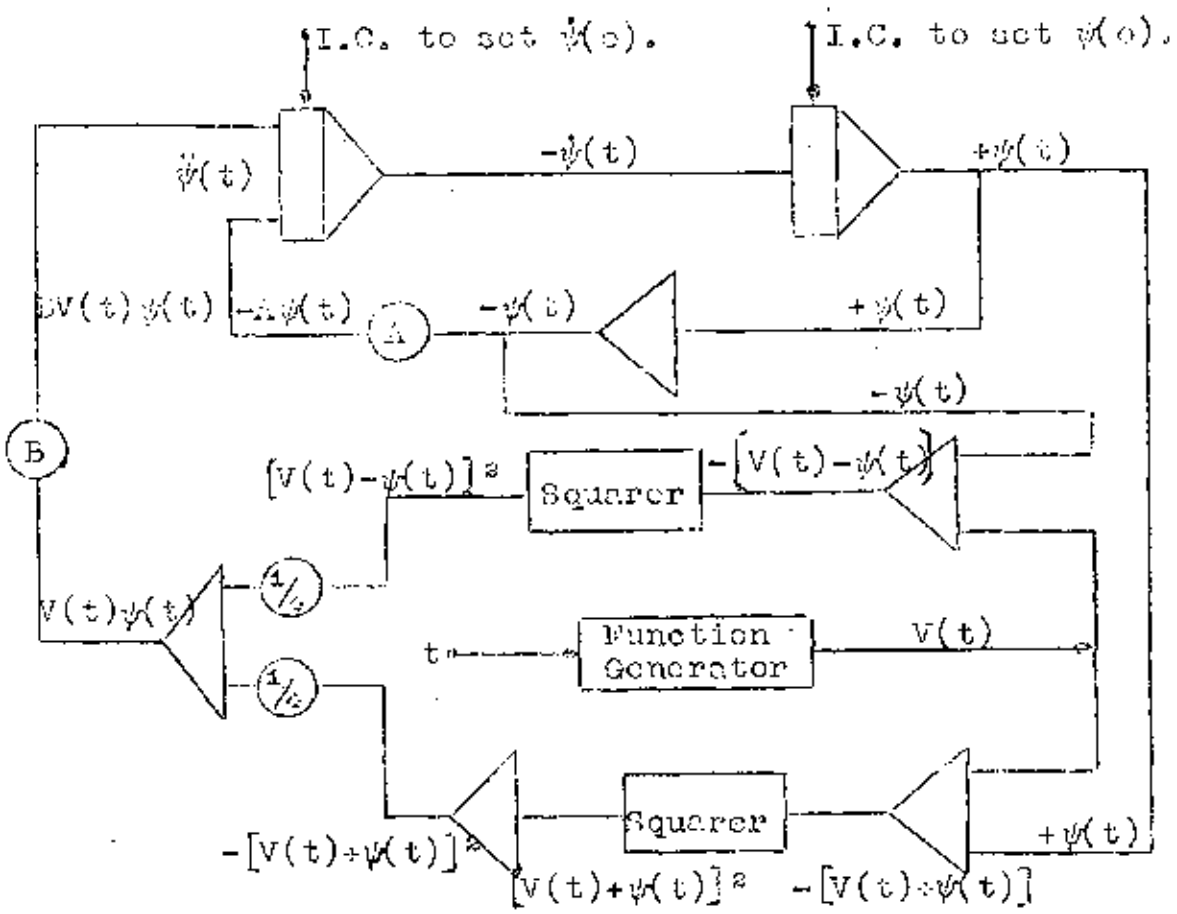


Fig.4.19: The Complete Computer Circuit for Equation (4.14).

The potential functions such as the potential step, the potential barrier, and the potential well, are constructed using straight line segments as we have explained in the chapter 2. The shapes which can be generated by the function generator are shown in Fig.4.20.

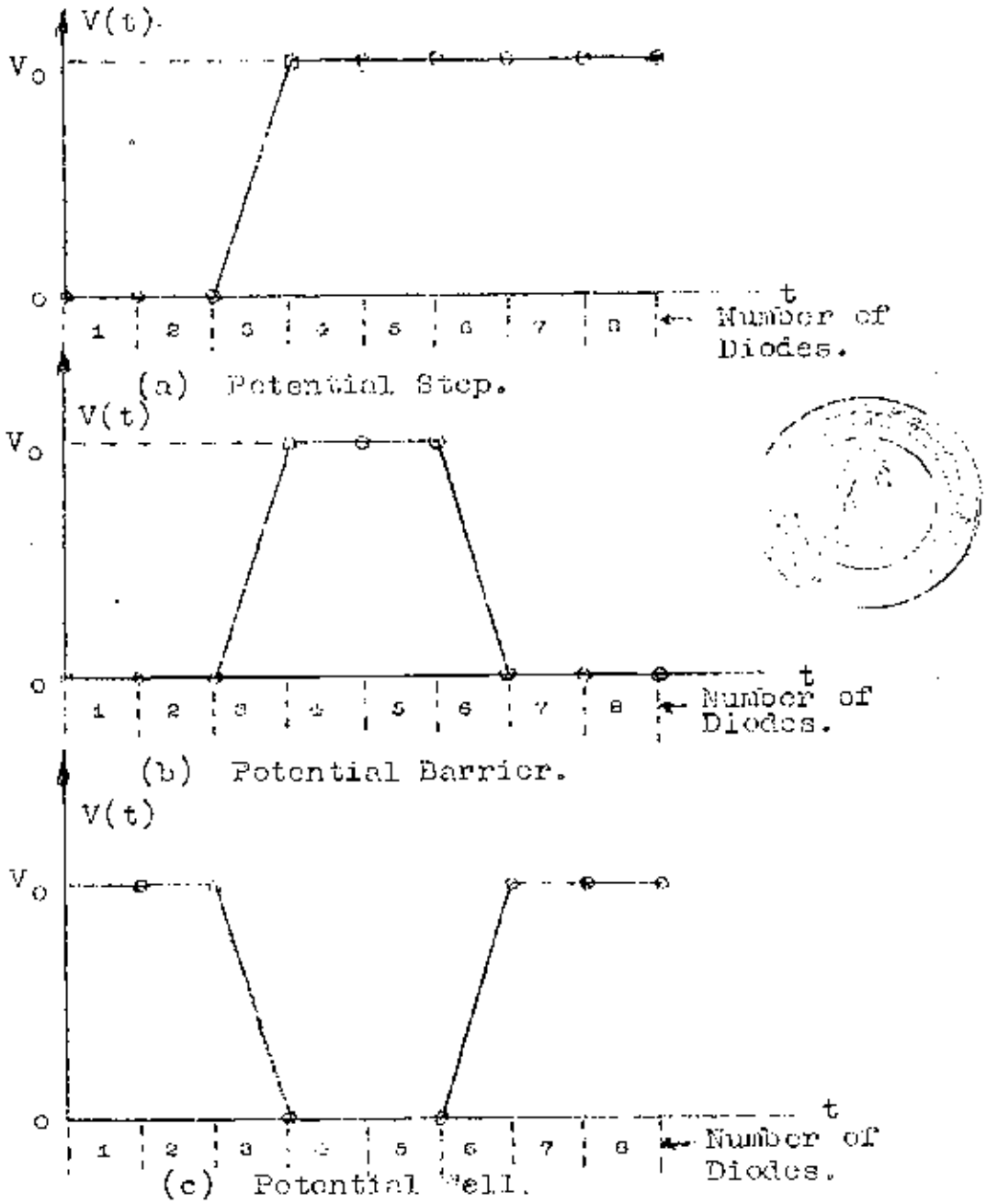


Fig.4.20: The Method of constructing the Potential Functions.

The procedures for operating the computer to obtain the solution in these cases are similar. Hence we will describe only one, the case of the potential step, as follows:

We will discuss the mathematical properties of the real wavefunctions which can be shown on the computer. The complex wavefunctions are ignored because they cannot be shown on the computer; details of them may be found in most books on quantum mechanics.[15] We will discuss the the potential step in two cases:

Case A: Given $E > V(t)$; Let E be the total energy of the particles, and Let $V(t)$ be the potential step shown in Fig.4.1b.

The time-independent Schrödinger equation in one-dimension for $t < t_0$ gives

$$\ddot{\psi}_1(t) + \frac{2mE}{\hbar^2}\psi_1(t) = 0 , \quad \text{--------- (4.16)}$$

and $$\psi_1(t) = A_1\cos p_1 t + A_2 \sin p_1 t , \; p_1 = \frac{\sqrt{2mE}}{\hbar} \text{---(4.17)}$$

For $t > t_0$ we have

$$\ddot{\psi}_2(t) + \frac{2m}{\hbar^2}(E-V_0)\,\psi_2(t) = 0 , \text{--------- (4.18)}$$

and $$\psi_2(t) = B_1\cos p_2 t + B_2 \sin p_2 t , \; p_2 = \frac{\sqrt{2m(E-V_0)}}{\hbar} \text{---(4.19)}$$

The real wavefunctions $\psi_1(t)$ and $\psi_2(t)$ represent the stationary waves produced by equal and opposite streams of particles.

At $t = t_0$, $V(t)$ is discontinuous. But since E, $V(t)$, and $\psi(t)$ are everywhere finite, it follows from the

Schrödinger equation that $\ddot{\psi}(t)$ is everywhere finite. Hence $\dot{\psi}(t)$ and $\psi(t)$ are finite and continuous everywhere, including $t = t_o$. Therefore at $t = t_o$ we have the boundary conditions $\psi_1(t_o) = \psi_2(t_o)$ and $\dot{\psi}_1(t_o) = \dot{\psi}_2(t_o)$. This gives two linear relations connecting the 4 constants A_1, A_2, B_1 and B_2. Eliminate B_1 and B_2 and put $B_1 = f(A_1, A_2)$ and $B_2 = g(A_1, A_2)$.

Then the complete real wavefunction over the whole region is defined by

$$\psi_1(t) = A_1 \cos p_1 t + A_2 \sin p_1 t \ , \ t \leq t_o . \text{---}(4.20)$$

$$\psi_2(t) = f(A_1, A_2) \cos p_2 t + g(A_1, A_2) \sin p_2 t, \ t \geq t_o \text{---}(4.21)$$

A_1 and A_2 may be chosen to represent any initial conditions $\psi(o)$ and $\dot{\psi}(o)$ on the computer.

The wavefunction for $E > V(t)$ is shown in Fig.4.21.

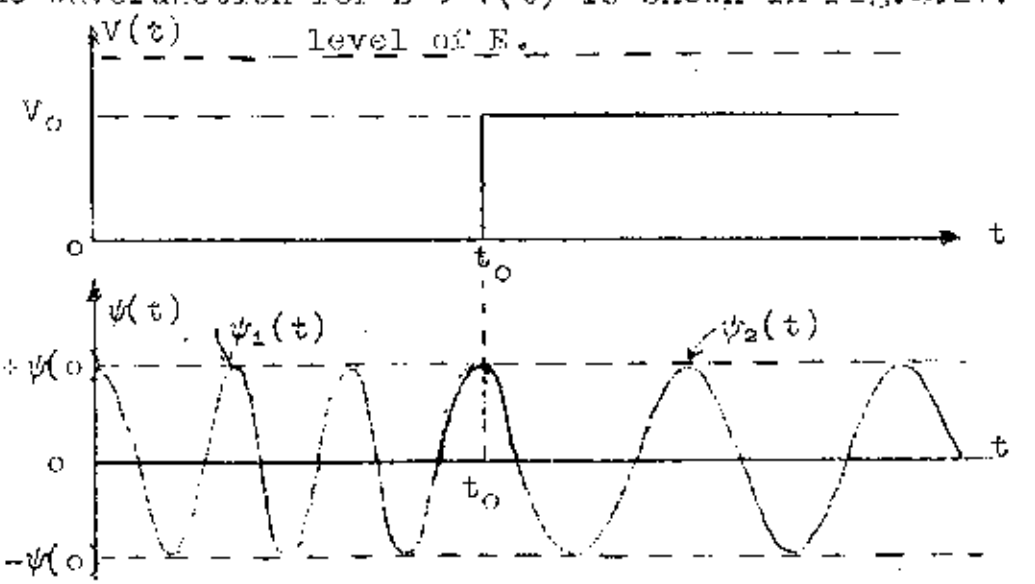


Fig.4.21: The Wavefunction of the Potential Step when $E > V(t)$.

In Fig.4.21, the wavelength in region $t < t_o$ is shorter than the wavelength in the region $t > t_o$, because the energy in the region $t < t_o$ is greater than the energy in the region $t > t_o$. Then the wavefunctions are in agreement with the de Broglie relation.

The boundary conditions at $t = t_o$ are automatically satisfied on the computer, and the initial conditions $\psi(o)$ and $\dot{\psi}(o)$ may be chosen freely. We can demonstrate this solution on the oscilloscope by the procedure as in caseII, merely by setting the potentiometer A to a large value and B to a small value.

Case.3: Given $0 < E < V_o$. Suppose that the kinetic energy of the particles is less than V_o, so that $E < V_o$. The Schrödinger equation is

$$\ddot{\psi}(t) - \frac{2m}{\hbar^2}(V_o - E)\,\psi(t) = 0. \quad \text{-------} \quad (4.22)$$

As before the wavefunction for $t < t_o$ is

$$\psi_1(t) = A_1 \cos p_1 t + A_2 \sin p_1 t\,, \quad p_1 = \frac{\sqrt{2mE}}{\hbar}\,, \quad \text{---} \quad (4.23)$$

and for $t > t_o$ is

$$\psi_2(t) = B_1 \exp.(p_2 t) + B_2 \exp.(-p_2 t), \quad p_2 = \frac{\sqrt{2m(V_o - E)}}{\hbar} \quad \text{--} (4.24)$$

Note that $\psi_2(t)$ is a combination of real exponentials. In order that the probability remain finite as $t \to +\infty$, it is necessary that we choose only the negative exponential,

i.e., that we choose $B_1 = 0$.

$$\therefore \quad \psi_2(t) = B_2 \exp.(-p_2 t) \quad \text{-------} \quad (4.25)$$

The density of particles to the right of the potential step is

$$|\psi_2(t)|^2 = |B_2|^2 \exp.(-2p_2 t) \quad \text{------} \quad (4.26)$$

Here the particle density $|\psi_2(t)|^2$ decays exponentially as t increases. The boundary conditions at $t = t_0$ are:

$\psi_1(t_0) = \psi_2(t_0)$ and $\dot{\psi}_1(t_0) = \dot{\psi}_2(t_0)$ as before.

This gives two linear relations:

$$\left.\begin{aligned} A_1 \cos p_1 t_0 + A_2 \sin p_1 t_0 &= B_2 \exp.(-p_2 t_0) \\ -A_1 p_1 \sin p_1 t_0 + A_2 p_1 \cos p_1 t_0 &= -B_2 p_2 \exp.(-p_2 t_0) \end{aligned}\right\} \quad \text{------(4.27)}$$

We have 3 arbitrary constants A_1, A_2, B_2 and two equations. Eliminate A_2 and B_2 and put $A_2 = f(A_1)$, $B_2 = g(A_1)$. Then the complete wavefunction over the whole region is defined by

$$\psi_1(t) = A_1 \cos p_1 t + f(A_1) \sin p_1 t \ , \quad t \leqslant t_0 \quad \text{--(4.28)}$$

$$\psi_2(t) = g(A_1) \exp.(-p_2 t) \ , \quad t \geqslant t_0 \ . \quad \text{------(4.29)}$$

A_1 may be chosen to represent the initial condition $\psi(0)$, but then $\dot{\psi}(0)$ must be set at the value to produce a satisfactory wavefunction that does not become infinite as

$t \to +\infty$.

The wavefunction in this case is shown in Fig. 4.22.

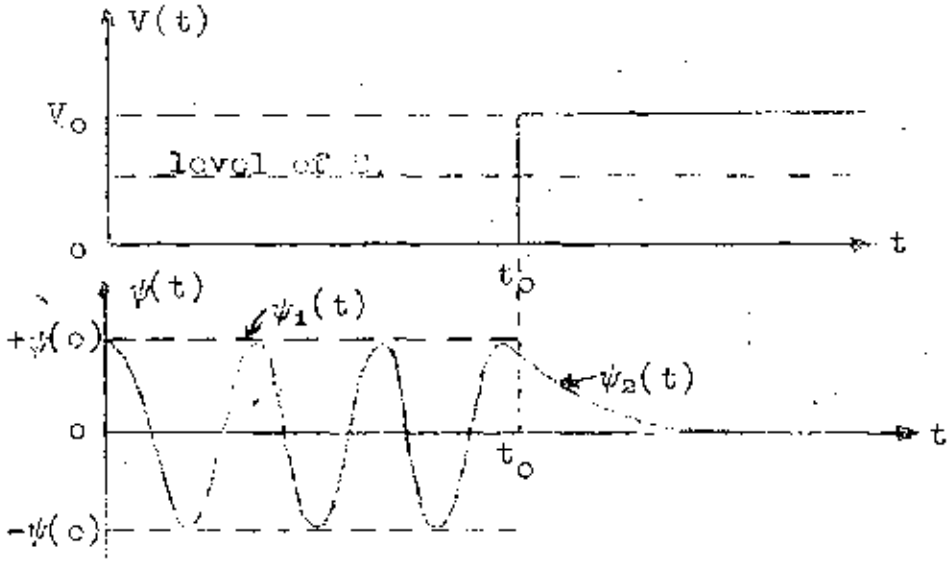


Fig. 4.22: The Wavefunction for the Potential Step when $E < V(t)$.

Again the boundary conditions at $t = t_o$ are automatically satisfied on the computer. We may obtain this solution on the oscilloscope by setting the potentiometer B to a large value and A to a small value, and fixing the value $\psi(o)$. Then adjust $\dot{\psi}(o)$ to make $\psi_2(t) = o$ when $t \to \infty$.

The physical interpretation of these solutions show that all the particles are reflected by the step. Their de Broglie waves of equal amplitude in opposite direction on the left of the step produce the standing wave shown on the oscilloscope. The "tail" for $t > t_o$ shows that some particles penetrate the potential step before being reflected.

We will not discuss the mathematical analysis in the cases of the potential barrier and the potential well. Details may be found in the literature.[16] We will discuss the physical interpretation of the wavefunctions which follow:

(a) Penetration of a Potential Barrier.

An eigenfunction for $E < V_o$ is shown in Fig.4.23.

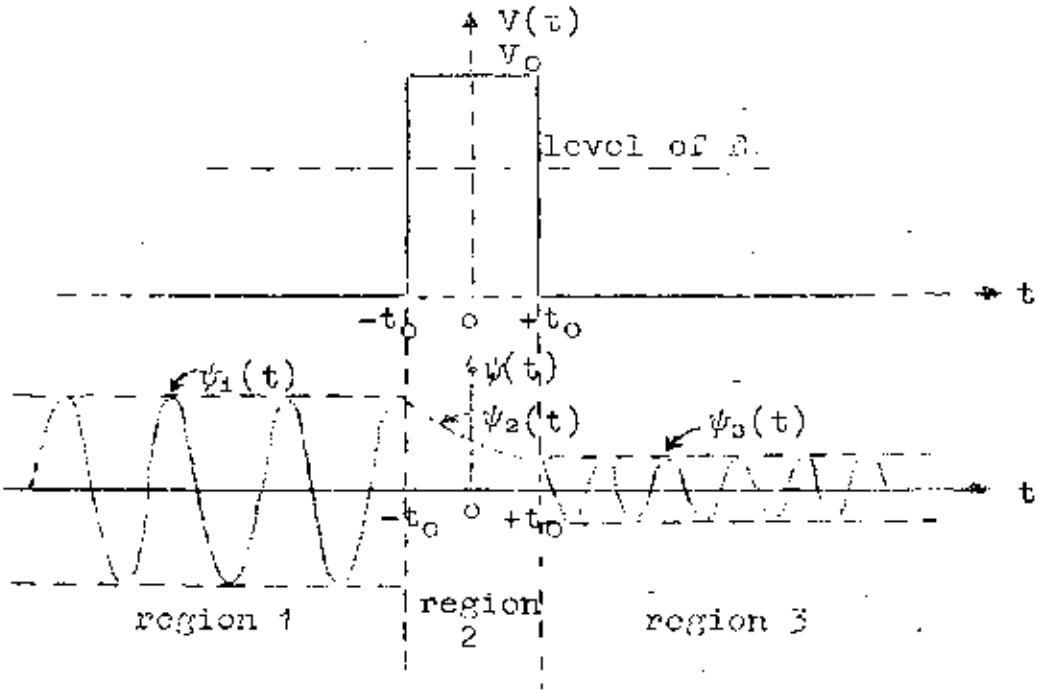


Fig.4.23: The wavefunction of the Potential Barrier when $E < V_o$.

This wavefunction shows how some particles may pass right through the barrier and emerges with their kinetic energy undiminished. The wavelengths in region 1 and 3 are the same because the particles have the same kinetic energy. The amplitude, which gives the particles density, is smaller in region 3.

(b) The Square-Well Potential.

In this case, when $E < V_0$ solutions are only found for certain values of E. These are the eigenvalues of E for the particle in the potential well. The solutions obtained are the eigenfunctions $\psi(t)$.

Let us consider a square-well potential. If for a particle in the well $E < V_0$ (See Fig.4.16) then there is a finite number of discrete levels which depends on the depth of the well. In the potential well the levels E_n are lower than the corresponding levels in a rigid box[17]; and there is always one more level with $E_n < V_0$, as shown in Fig.4.24.

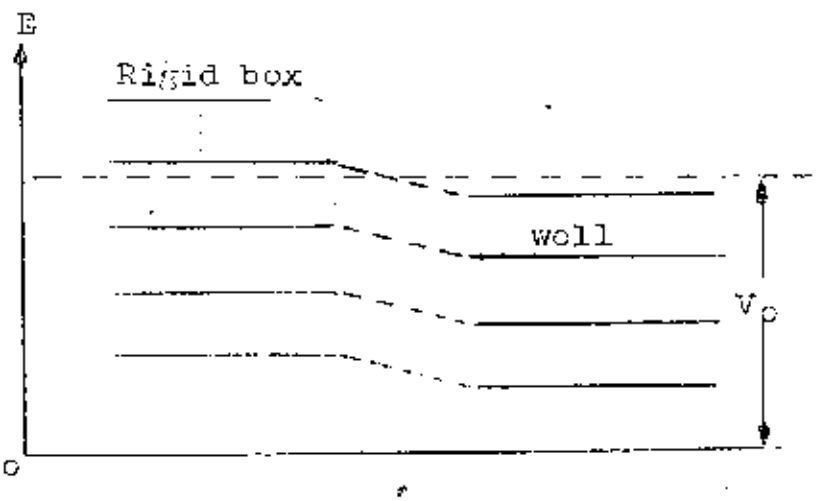


Fig.4.24: The Discrete Energy Levels.

Possible eigenfunctions for $E < V_0$ are illustrated in Fig.2.25.

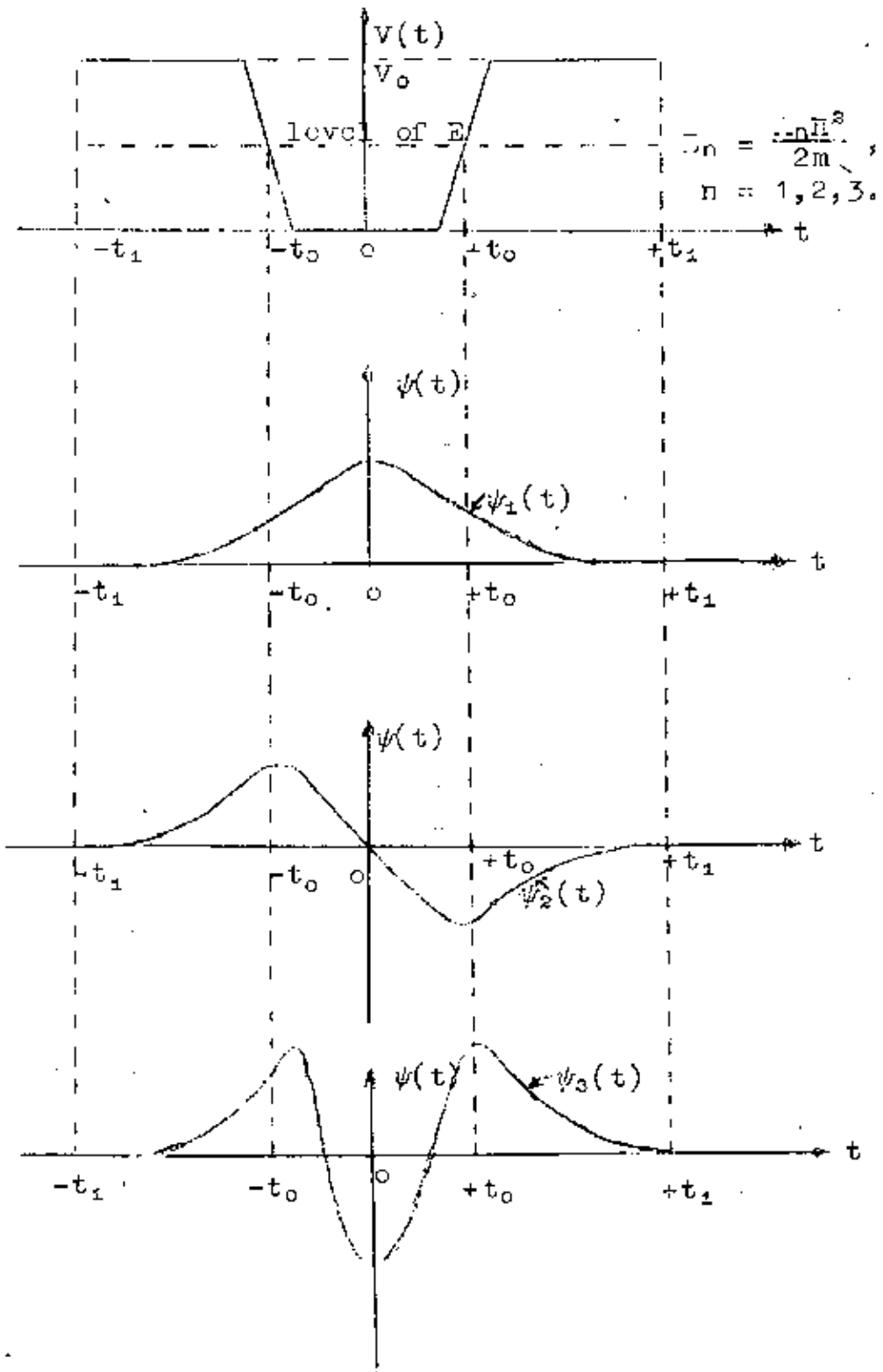


Fig.4.25: The lowest energy eigenfunctions for the well when $E < V_o$.

We now consider the bound states of the square well. When $t < -t_0$ [see $\psi_1(t)$], the exponential solution is increasing with increasing t and curving upward. At $t = -t_0$, the kinetic energy becomes positive and, since $\psi(t)$ is positive, $\ddot{\psi}(t)$ becomes negative. Then the wavefunction begins to curve back toward the t-axis, at a rate depending on V_0-E. When $t > t_0$, 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. Thus, only certain values of E will lead to bound states. These will be the eigenvalues.

If V_0 is very large, then $\psi(t)$ can fit onto the decaying exponential at $t = +t_0$ after one or more oscillations. The first few possibilities are illustrated in $\psi_2(t)$ and $\psi_3(t)$.

To obtain the eigenfunction on an analogue computer, we start by setting the initial condition $\psi(o) = 0$ at $t = -t_1$ and let $\dot{\psi}(o)$ vary. We adjust $\dot{\psi}(o)$ and potentiometer A to try and get a solution which approximates $\psi(t)$ zero at $t = +t_1$. Then we obtain the eigenfunctions and the eigenvalues.

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