CHAPTER III.

AN OUTLINE OF SCHRÖDINGER EQUATION

In the previous chapter, we discussed the operation of an analogue computer. In order to demonstrate the solution of Schrödinger's equation on an analogue computer, it is necessary to know about Schrödinger's equation. In this chapter we will give a very brief introduction to the Schrödinger wave theory of a particle.

The principal equation in quantum mechanics is Schrödinger's equation. The well known time-independent Schrödinger equation for a single particle in one-dimension, is as follows.(5),(10).

$$\frac{d^2\psi(x)}{dx^2} + \frac{2m}{\hbar^2}\left[E-V(x)\right]\psi(x) = 0 \qquad \text{------} \quad (3.1)$$

where $\psi(x)$ is the wavefunction,

E is the total energy,

$V(x)$ is the potential energy function,

m is the mass of the particle,

and $2\pi\hbar$ is Planck's constant (6.625×10^{-27} erg.sec.).

The wavefunction $\psi(x)$ represents the behaviour of the particle in the potential field $V(x)$. $/\psi(x)/^2dx$ is the probability of finding the particle in the interval x to $x+dx$. The mathematical properties of wavefunctions with a satisfactory physical interpretation are: $\psi(x)$ is finite, single-valued, and continuous. For a single particle $\psi(x)$ is so chosen that $\int_{-\infty}^{+\infty}|\psi(x)|^2 dx = 1$, since the probability of finding the particle somewhere on the x-axis is unity. Further-more, $\psi(x)$ may also represent a stream of particles of infinite extent on the x-axis. In this case $\psi(x)$ is also chosen that $|\psi(x)|^2$ represents the density of particles in the stream. Here $\int_{-\infty}^{+\infty}|\psi(x)|^2 dx = +\infty$, since there are infinitely many particles on the whole x-axis.

Equation (3.1) is the Schrödinger equation whose solutions are to be demonstrated on the analogue computer. It will be possible to illustrate many important effects peculiar to quantum mechanics, such as the penetration of a potential barrier, the reflection of the de Broglie[11] wave of a particle by a sharp change in potential, and the discrete energy states of a particle bound in a narrow region by an attractive force. The Schrödinger equation is applied to various physical systems by inserting the appropriate potential function V(x), and finding the solutions $\psi(x)$ that are finite, single-valued, and continuous. The potential functions we shall discuss later are the following:

(3.1) The Free Particle.

When no force acts on the particle we may put the potential function V(x) = 0 for all x. Since V(x) is also independent of the time, Schrödinger's time-independent equation takes the form

$$\frac{d^2\psi(x)}{dx^2} + \frac{2m}{\hbar^2} E\ \psi(x) = 0 \qquad \text{------------} \quad (3.2)$$

(3.2) The Constant Potential.

In this case the potential function has a constant value and we may put $V(x) = V_0$ for all x. The time-independent Schrödinger equation in one-dimension is

$$\frac{d^2\psi(x)}{dx^2} + \frac{2m}{\hbar^2}(E-V_0)\ \psi(x) = 0 \qquad \text{----------} \quad (3.3)$$

(3.3) The Potential Step.

The potential energy is a step function defined by

$$\left.\begin{array}{llll} V(x) = 0 & , & x < x_0 , \\ V(x) = V_0 & , & x > x_0 . \end{array}\right\} \qquad \text{--------} \quad (3.4)$$

The potential step is shown in Fig.3.1.

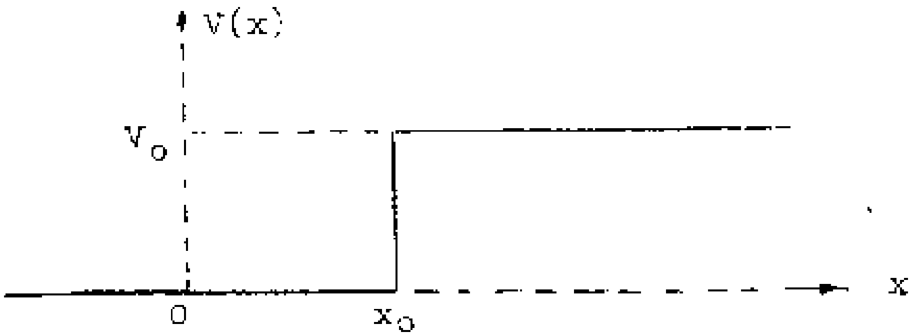

Fig.3.1: The Potential Step.

The time-independent Schrödinger equation for $x < x_o$ is the same as equation (3.2), and for $x > x_o$ is the same as equation (3.3).

(3.4) The Potential Barrier.

In this problem the potential function is defined by

$$\left.\begin{array}{lll} V(x) = 0 & , & x < o , \\ V(x) = V_o & , & o \leqslant x \leqslant x_o , \\ V(x) = 0 & , & x > x_o . \end{array}\right\} \qquad \text{------} \quad (3.5)$$

We have a potential barrier between $x = o$ and $x = x_o$, as shown in Fig.3.2.

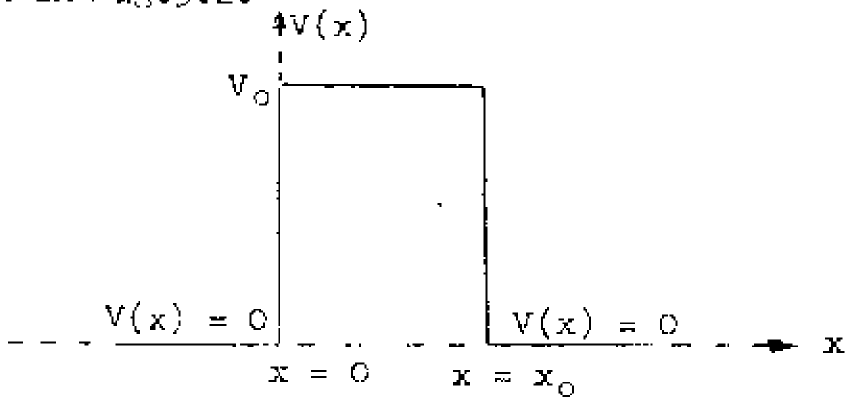

Fig.3.2: The Potential Barrier.

(4.5) The Square-Well Potential.

Let us consider a square-well potential defined by

$$\left.\begin{array}{lll} V(x) = V_o & , & x < -x_o , \\ V(x) = 0 & , & -x_o \leqslant x \leqslant +x_o , \\ V(x) = V_o & , & x > +x_o . \end{array}\right\} \qquad \text{-----} \quad (3.6)$$

The square-well potential is shown in Fig.3.3.

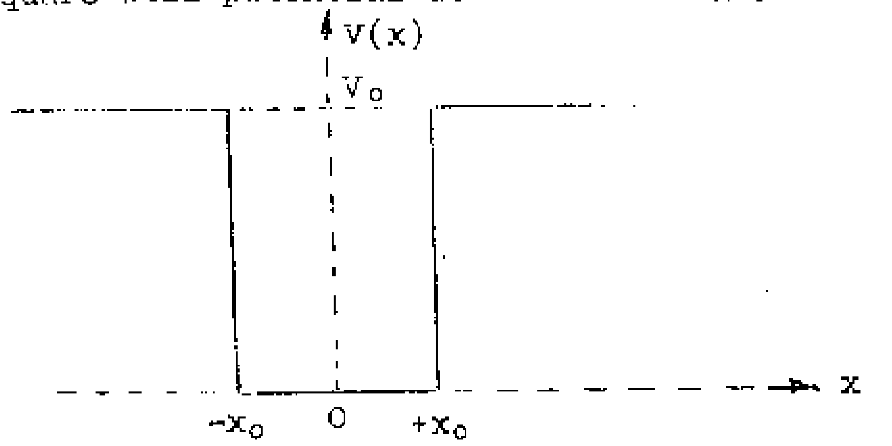

Fig.3.3: The Square-Well Potential.

The solutions for each case will be given later.

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