$$\frac{E}{V_0}$$

It may be noted here that if V_0 is replaced in the problem by $-V_0$, the potential well problem becomes the problem of a potential barrier of barrier height V_0 and width L. The case of potential well of depth V_0 with particle energy $E > 0$ becomes analogous to the case of potential barrier of height V_0 with particle energy $E + V_0$. Therefore, it may be easily checked that the expressions for R and T [Eqs. (5.112) may be obtained from Eqs. (5.94) simply by replacing V_0 by $-V_0$].

A schematic plot of T as a function of E/V_0 will show similar behaviour as that shown in Figure 5.1.

5.9 KRONIG–PENNEY MODEL

In previous sections, we have studied energy eigenvalues and eigenfunctions of a particle in simple one-dimensional potentials of various forms: potential box, potential well, potential step, and so on. In many situations, we encounter a situation where a particle is moving in a periodic potential. For example, in case of metal or semiconductor, where the crystal structure is periodic, the electrons experience a periodic potential. So while discussing the conduction or insulation properties of the solids, we should have the knowledge of what are energy eigenvalues and eigenstates of electrons in the periodic potential of these solids. Let us consider a one-dimensional crystalline solid (say a metal) with positive ions forming a one-dimensional array of lattice parameter a (shown in Figure 5.17). The resultant potential of all ions, which an electron feels, is periodic and is shown schematically in the figure. When the electron reaches at the boundary (of the one-dimensional solid), it feels a high potential which gives rise to the work-function of metals.

If we ignore the potential rise at the two boundaries, the potential is periodic throughout and has the property $V(x) = V(x + na)$, here n is an integer. Kronig and Penney suggested a very simple (one-dimensional) potential function which is periodic and has qualitative features of the potential shown in Figure 5.17. The potential, known as Kronig–Penney potential, is shown in Figure 5.18.
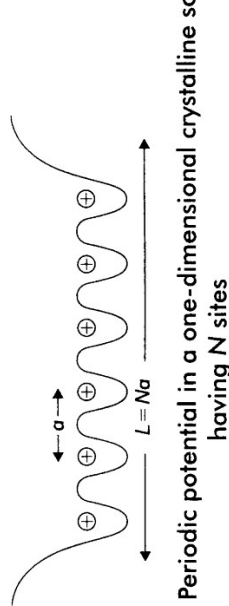
Figure 5.17 Periodic potential in a one-dimensional crystalline solid having N sites
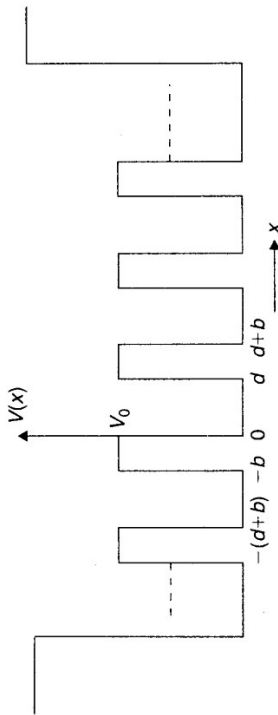
Figure 5.18 The Kronig-Penney potential with periodicity $a(= d + b)$; d being width of the well and b the width of (rectangular) potential barrier of height V_0.

$$\frac{2m(V_0 + E)}{\hbar^2}\left(\frac{L}{2}\right)^2 = (n+1)^2 \left(\frac{\pi}{2}\right)^2$$

$$E = -V_0 + \frac{(n+1)^2 \pi^2 \hbar^2}{2mL^2} \tag{5.110}$$

This result is the same as that obtained in Section 5.4 for a particle in a potential box (i.e., a potential well of infinite depth). We may note here that $E + V_0$ [$= (n+1)^2 \pi^2 \hbar^2 / 2mL^2$] is the distance in energy from the bottom of the well and, therefore, represents the kinetic energy of the particle in the well.

5.8.2 Case II: $E > 0$

We now turn to the case when the particle, in connection with potential well of Figure 5.14 is having positive energy and, therefore, the particle is not bound in the potential well. Considering the particle being incident upon the well from the left, the solutions of the Schrodinger equation in regions I, II, and III, respectively, are given by

$$\psi(x) = Ae^{ikx} + Be^{-ikx}, \qquad x < -L/2 \tag{5.111}$$

$$\psi(x) = Fe^{ik_1 x} + Ge^{ik_1 x}, \qquad L/2 < x < L/2 \tag{5.111}$$

$$\psi(x) = Ce^{ikx}, \qquad x > L/2 \tag{5.111}$$

with

$$k = \sqrt{\frac{2mE}{\hbar^2}}, \qquad k_1 = \sqrt{\frac{2m(V_0 + E)}{\hbar^2}},$$

It may be noted that in the region I ($x < -L/2$), the wave function consists of an incident wave of amplitude A and a reflected wave of amplitude B, while in region III ($x > L/2$), the wave function consists of only a pure transmitted wave of amplitude C.

The constants A, B, C, F, and G appearing in Eqs (5.111) can be related by the requirement of the continuity of $\psi(x)$ and $d\psi/dx$ at the two boundaries $x = \pm L/2$. We may note that this continuity of $\psi(x)$ may be realized for any value of E (>0), so all (continuous) values of E (>0) are allowed energy eigenvalues. Proceeding in the same way as, for example, in Section 5.7, one can solve for the ratios B/A and C/A and one may get expressions of reflection coefficient $R = |B/A|^2$ and transmission coefficient $T = |C/A|^2$, as

$$R = \left[1 + \frac{4k^2 k_1^2}{(k - k_1^2)^2 \sin^2 k_1 L}\right]^{-1} = \left[1 + \frac{4E(V_0 + E)}{V_0^2 \sin^2 k_1 L}\right]^{-1} = \left[1 + \frac{4\epsilon(1 + \epsilon)}{\sin^2\left(\sqrt{2\alpha(1 + \epsilon)}\right)}\right]^{-1} \tag{5.112}$$

$$T = \left[1 + \frac{(k^2 - k_1^2)\sin^2 k_1 L}{4k^2 k_1^2}\right]^{-1} = \left[1 + \frac{V_0^2 \sin^2 k_1 L}{4E(V_0 + E)}\right]^{-1} = \left[1 + \frac{\sin^2\left(\sqrt{2\alpha(1 + \epsilon)}\right)}{4\epsilon(1 + \epsilon)}\right]^{-1} \tag{5.112}$$

5.1 Case-I: $E < V_0$

To find out energy eigenvalues and eigenstates of a particle in the periodic potential (Figure 5.1) we shall have to solve Schrodinger equation

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}[E - V(x)]\psi(x) = 0 \tag{5.11?}$$

with

$$V(x) = 0 \quad \text{for} \quad 0 < x < d$$
$$V(x) = V_0 \quad \text{for} \quad d < x < (d+b) \tag{5.11?}$$

and

$$V(x) = V(x+a) \tag{5.11?}$$

We notice that the periodic property of $V(x)$ [Eq. (5.115)] may not be realized at the two ends of th... lattice. It is a fact that there are a very large number of ion sites in the sample of a one-dimensional sol... and, therefore, the effect of potential rise at the two boundaries hardly affects the transport behavio... of the electrons inside. In our treatment of finding eigenstates of electron in potential of Figure 5.1... boundary effects can be avoided if we use periodic boundary conditions (discussed in Section 5.6) ... the wave function:

$$\psi(x+L) = \psi(x) \tag{5.11?}$$

In fact the use of periodic boundary conditions is one way of getting rid of the effects of the boundarie... Now the solution $\psi(x)$ of the one-dimensional Schrodinger [Eq. (5.113)] for a periodic potent... [Eq. (5.114)], according to Bloch theorem (see Appendix B3), is of the form

$$\psi(x) = e^{ikx}u(x) \tag{5.11?}$$

where k is arbitrary (wave vector) and $u(x)$ has the periodicity of the potential $V(x)$, that is,

$$u(x+a) = u(x) \tag{5.11?}$$

Applying the periodic boundary conditions [Eq. (5.116)] on the wave function $\psi(x)$ [Eq. (5.117)] we get

$$\psi(x+L) = \psi(x+\tilde{N}a) = e^{ik(x+Na)}u(x+Na)$$
$$= e^{ikNa}e^{ikx}u(x)$$
$$= e^{ikNa}\psi(x) \tag{5.119}$$

Comparing Eq. (5.119) with Eq. (5.116), we get

$$e^{ikNa} = 1$$

or

$$k = (say)\ k_n = \frac{2n\pi}{Na} = \frac{2n\pi}{L} \tag{5.120}$$

We now turn to solving Schrodinger equation.

The general solution of Schrodinger equation in the potential well region ($0 < x < d$) is

$$\psi_I(x) = Ae^{ik_1x} + Be^{-ik_1x}$$
$$\frac{\hbar^2 k_1^2}{2m} = E$$

The wave function in the barrier region ($-b \leq x \leq 0$) is

$$\psi_{II}(x) = Ce^{ik_2x} + De^{-ik_2x}$$
$$\frac{\hbar^2 k_2^2}{2m} = (E - V_0)$$

The complete solution $\psi_I(x)$ and $\psi_{II}(x)$ should have the Bloch form [Eq. (5.117)]. From Bloch theo...

$$\psi(x+a) = e^{i(x+a)}u(x+a)$$
$$= e^{ikx}u(x)e^{ika} \quad [\text{as}\ u(x+a) = u(x)]$$
$$= \psi(x)e^{ika}$$

Thus taking x in the interval $(-b, 0)$ (i.e., for $-b \leq x \leq 0$) we have $(x+a)$ lying in the interval (d... (i.e., $d < x < a$), so

$$\psi(d < x < a) = \psi(-b < x < 0)e^{ika} \tag{5.11?}$$

The wave function $\psi(x)$ and its derivative $d\psi/dx$ should be continuous at $x = 0$ and $x = d$. The boundary conditions should be used to determine the constants A, B, C, and D appearing in Eqs (5.1... Eq. (5.12?). Using these conditions at $x = 0$ give

$$A + B = C + D$$
$$k_1(A - B) = k_2(C - D)$$

Condition (5.124) dictates that the wave function at $x = d$ is related with the wave function at x ... the following way

$$\psi_I(x = d) = \psi_{II}(x = -b)e^{ika} \tag{5.11?}$$

Also their derivatives are related as

$$\frac{d\psi_I}{dx}\Big|_{x=d} = \frac{d\psi_{II}}{dx}\Big|_{x=-b}e^{ika}$$

These two equations give

$$Ae^{ik_1d} + Be^{-ik_1d} = (Ce^{-ik_2b} + De^{ik_2b})e^{ika}$$
$$k_1(Ae^{ik_1d} - Be^{-ik_1d}) = k_2(Ce^{-ik_2b} - De^{ik_2b})e^{ika}$$

The four Eqs (5.125) and (5.128) may be written in the matrix form:

$$\begin{bmatrix} 1 & 1 & -1 & -1 \\ k_1 & -k_1 & -k_2 & k_2 \\ e^{ik_1d} & e^{-ik_1d} & -e^{ika}e^{-ik_2b} & -e^{ika}e^{ik_2b} \\ k_1e^{ik_1d} & -k_1e^{-ik_1d} & -k_2e^{ika}e^{-ik_2b} & k_2e^{ika}e^{ik_2b} \end{bmatrix}\begin{bmatrix} A \\ B \\ C \\ D \end{bmatrix} = 0$$

Equation (5.129) has nontrivial solution only if the determinant of the 4×4 matrix vanishes, leads to the following equation (the dispersion relation) as can be checked by doing a but lengthy straightforward algebra.

dispersion relation for $E > V_0$ case can be easily obtained from Eq. (5.130) simply by the replace... ik_2, κ

dispersion relation comes out to be

$$\cos k_1 d \cos \kappa b - \frac{k_1^2 - \kappa^2}{2k_1\kappa}\sin k_1 d \sinh \kappa b = \cos k(d+b) \tag{5.1}$$

with

$$k_1 = \frac{\sqrt{2mE}}{\hbar}, \quad \kappa = \frac{\sqrt{2m(V_0 - E)}}{\hbar}, \quad k_1^2 + \kappa^2 = \frac{2mV_0}{\hbar^2} \tag{5.1}$$

...(5.130) and (5.134) are transcendental and, therefore, can be solved only numerically t... ...relations $E(k)$, that is, to find allowed values of E for given values of wave vectors k. In t... ...the right hand sides of both Eqs (5.130) and (5.134) have values only within the interval $[+1, ...$ ...within the interval $[+1, -1]$. So only those values of E are possible for which left hand sides of these equation... ...that is, $\cos ka$ [with allowed values of k as $k_n = 2n\pi/Na$ Eq. (5.120)] has only discrete l... ...the interval $[+1, -1]$. This aspect is shown on the left part of Figure 5.19, where horizontal lines... ...atically, the allowed values of $\cos ka$. On the right part of Figure 5.19, the horizontal lines (in the left part... ...band values of Eqs (5.130) and (5.134) as a function of E/V_0. The horizontal lines (in the left part... ...may be imagined to be extending towards right side and wherever these cut the curve, we... ...of energy eigenvalues. For example, these lines cut the curve in between the points a and b... ...and so on. So the energy eigenvalues lie in the intervals $[a', b']$, $[c', d']$, $[e', f']$, and so on. The... ...of energy bands, separated by band gaps. In Figure 5.20, we show schematic plot of allowed... ...allowed values E as a function of wave vector k, obtained from the graphical solution shown in Figure 5.19.

5.9.2 Case-II: $E < V_0$

For the case $E < V_0$, the general solution of Schrodinger equation in the potential well region rem... the same as Eq. (5.121). But in the barrier region the solution takes the form

$$\psi_{II}(x) = Ce^{\kappa x} + De^{-\kappa x}$$

where

$$\frac{\hbar^2 \kappa^2}{2m} = (V_0 - E)$$

$$\cos k_1 d \cos k_2 b - \frac{k_1^2 + k_2^2}{2k_1 k_2}\sin k_1 d \sin k_2 b = \cos k(d+b)$$

$$k_1 = \frac{\sqrt{2mE}}{\hbar}, \quad k_2 = \frac{\sqrt{2m(E-V_0)}}{\hbar}, \quad k_1^2 - k_2^2 = \frac{2mV_0}{\hbar^2}$$
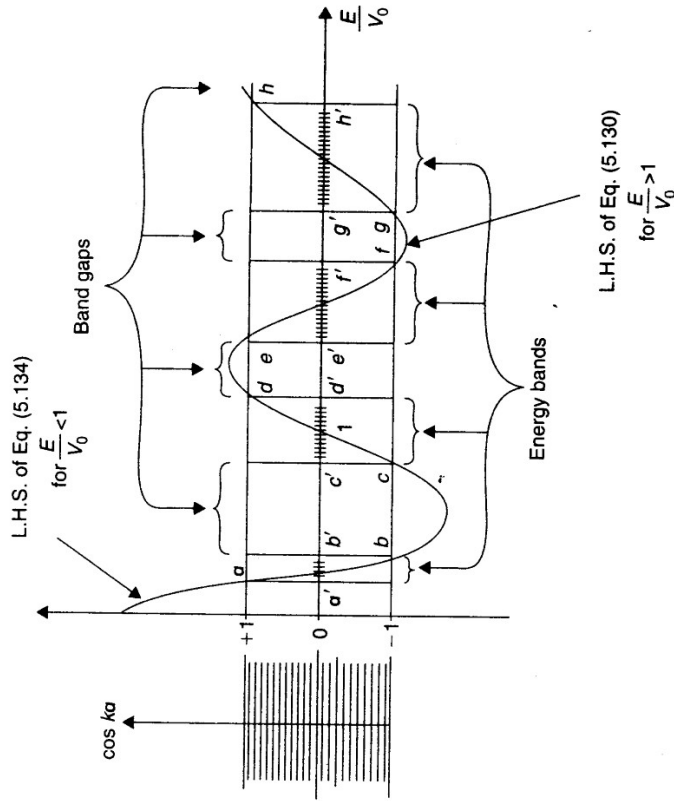

Figure 5.19 Schematic plot of L.H.S. of Eq. (5.134) [for $(E/V_0) < 1$] and of Eq. (5.130) [for $(E/V_0) > 1$] as a function of (E/V_0). The two horizontal lines at ordinates $+1$ and -1 are the two extreme values of (E/V_0). On the left hand part of the figure we show (schematically) the allowed values of $\cos ka$, where $k = k_n = 2n\pi/Na$ Eq. (5.120)
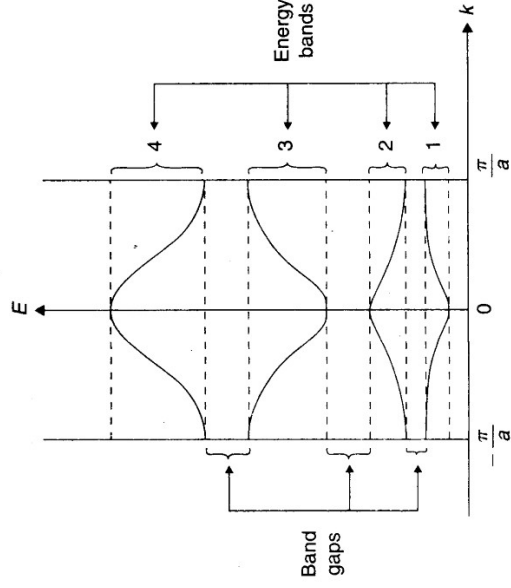

Figure 5.20 Schematic plot of allowed energy eigenvalues E as a function of wave vector k, obtained from the graphical solution shown in Figure 5.19. The energy bands shown as 1, 2, 3, 4 correspond to allowed energy values in the intervals $[a', b']$, $[c', d']$, $[e', f']$ and $[g', h']$ respectively of Figure 5.19