KITTEL 2nd Ed.

we have

(11.11) $$\psi_k = e^{ikx}u_k(x),$$

which is the Bloch result.

KRONIG-PENNEY MODEL

We demonstrate some of the characteristic features of electron propagation in crystals by considering the periodic square-well structure[4] in one dimension (Fig. 11.7). This is a highly artificial model,

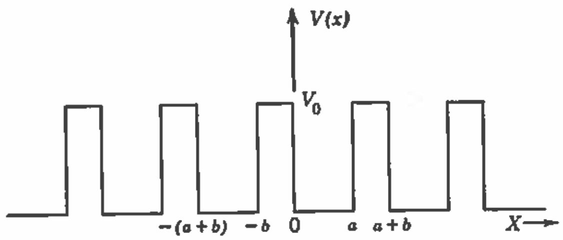

Fig. 11.7. Kronig and Penney one-dimensional periodic potential.

but it is a model which can be treated explicitly, using only elementary functions. The wave equation of the problem is

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

The running wave solutions will be of the form of a plane wave modulated with the periodicity of the lattice. Using (11.11), we obtain solutions of the form

(11.13) $$\psi = u_k(x)e^{ikx},$$

where $u(x)$ is a periodic function in x with the period $(a + b)$ and is determined by substituting (11.13) into (11.12):

(11.14) $$\frac{d^2u}{dx^2} + 2ik\frac{du}{dx} + \frac{2m}{\hbar^2}(E - E_k - V)u = 0,$$

where $E_k = \hbar^2k^2/2m$.

In the region $0 < x < a$ the equation has the solution

(11.15) $$u = Ae^{i(\alpha-k)x} + Be^{-i(\alpha+k)x},$$

[4] R. de L. Kronig and W. G. Penney, Proc. Roy. Soc., (London) **A130**, 499 (1931); see also D. S. Saxon and R. A. Hutner, Philips Research Repts. **4**, 81 (1949); J. M. Luttinger, Philips Research Repts. **6**, 303 (1951).

provided that

$$\alpha = (2mE/\hbar^2)^{1/2}. \tag{11.16}$$

In the region $a < x < a + b$ the solution is

$$u = Ce^{(\beta - ik)x} + De^{-(\beta + ik)x}, \tag{11.17}$$

provided that

$$\beta = [2m(V_0 - E)/\hbar^2]^{1/2}. \tag{11.18}$$

The constants A, B, C, D are to be chosen so that u and du/dx are continuous at $x = 0$ and $x = a$, and by the periodicity required of $u(x)$ the values at $x = a$ must equal those at $x = -b$. Thus we have the four linear homogeneous equations:

$$A + B = C + D;$$

$$i(\alpha - k)A - i(\alpha + k)B = (\beta - ik)C - (\beta + ik)D;$$

$$Ae^{i(\alpha - k)a} + Be^{-i(\alpha + k)a} = Ce^{-(\beta - ik)b} + De^{(\beta + ik)b}$$

$$i(\alpha - k)Ae^{i(\alpha - k)a} - i(\alpha + k)Be^{-i(\alpha + k)a} = (\beta - ik)Ce^{-(\beta - ik)b} - (\beta + ik)De^{(\beta + ik)b}.$$

These have a solution only if the determinant of the coefficients vanishes, or[5]

$$\frac{\beta^2 - \alpha^2}{2\alpha\beta} \sinh \beta b \sin \alpha a + \cosh \beta b \cos \alpha a = \cos k(a + b). \tag{11.19}$$

In order to obtain a handier equation we represent the potential by a periodic delta function, passing to the limit where $b = 0$ and $V_0 = \infty$ in such a way that $\beta^2 b$ stays finite. We set

$$\lim_{\substack{b \to 0 \\ \beta \to \infty}} \frac{\beta^2 ab}{2} = P, \tag{11.20}$$

so that the condition (11.19) becomes

$$P \frac{\sin \alpha a}{\alpha a} + \cos \alpha a = \cos ka. \tag{11.21}$$

This transcendental equation must have a solution for α in order for wave functions of the form (11.13) to exist.

[5] Before verifying this for himself the reader should refer to the alternative derivation in the following section.

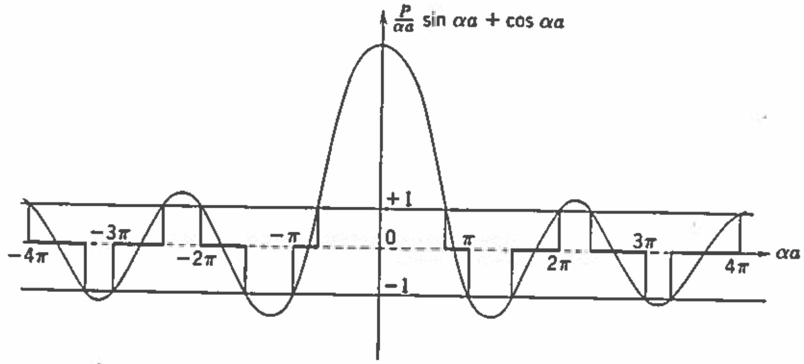

Fig. 11.8. Plot of the function $P\frac{\sin \alpha a}{\alpha a} + \cos \alpha a$, for $P = 3\pi/2$. The allowed values of the energy E are given by those ranges of $\alpha = [2mE/\hbar^2]^{1/2}$ for which the function lies between +1 and −1. (After Kronig and Penney.)

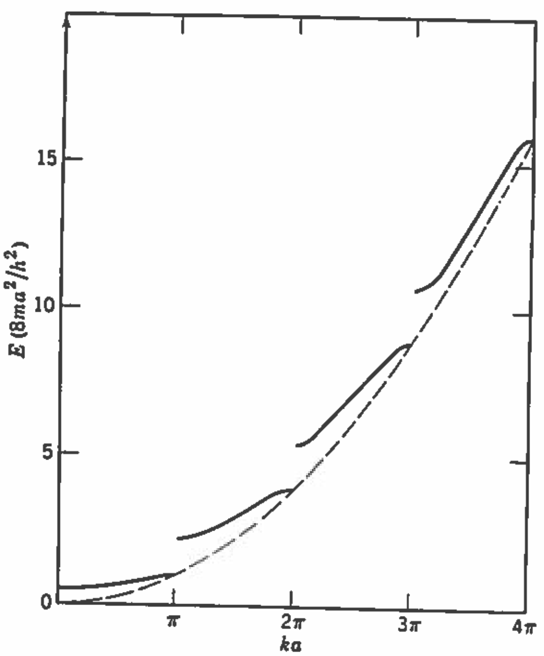

Fig. 11.9. Plot of energy vs. wave number for the Kronig-Penney potential, with $P = 3\pi/2$. (After Sommerfeld and Bethe.)

In Fig. 11.8 we have plotted the left side of (11.21) as a function of αa, for the arbitrary value $P = 3\pi/2$. As the cosine term on the right side can have values only between $+1$ and -1, only those values of αa are allowed for which the left side falls in this range. The allowed ranges of αa are drawn heavily in the figure, and through the relation $\alpha = [2mE/\hbar^2]^{1/2}$ they correspond to allowed ranges of the energy E. The boundaries of the allowed ranges of αa correspond to the values $n\pi/a$ for k. In Fig. 11.9 E vs. k is plotted.

If P is small, the forbidden ranges disappear. If $P \to \infty$, the allowed ranges of αa reduce to the points $n\pi$ $(n = \pm 1, \pm 2, \cdots)$. The energy spectrum becomes discrete, and the eigenvalues

$$E = n^2h^2/8ma^2$$

are those of an electron in a box of length a.

ALTERNATIVE DERIVATION OF THE KRONIG-PENNEY RESULT

We derive here by a direct method the result (11.21) for the delta-function potential array, avoiding the very considerable labor incident to (11.19). We note first that in the region under the delta-function $\beta \gg k$, so that d^2u/dx^2 is much larger than du/dx in this region. Our boundary conditions are then that in the limit of a delta-function potential the value of u is continuous through the potential, or, using the periodicity condition,

$$A + B \cong Ae^{i(\alpha-k)a} + Be^{-i(\alpha+k)a}; \tag{11.22}$$

furthermore, the derivatives are related by

$$\begin{aligned}(du/dx)_a &\cong (du/dx)_0 - (d^2/dx^2)_0 b \cong (du/dx)_0 - b\beta^2 u(0) \\ &= (du/dx)_0 - (2P/a)u(0),\end{aligned} \tag{11.23}$$

where P is defined by (11.20). Therefore

$$\begin{aligned}&[i(\alpha - k) - (2P/a)]A - [i(\alpha + k) + (2P/a)]B \\ &\qquad = i(\alpha - k)Ae^{i(\alpha-k)a} - i(\alpha + k)e^{-i(\alpha+k)a}B.\end{aligned} \tag{11.24}$$

The determinantal equation for the existence of a solution of (11.22) and (11.24) is

$$\begin{vmatrix} 1 - e^{i(\alpha-k)a} & 1 - e^{-i(\alpha+k)a} \\ i(\alpha-k)(1-e^{i(\alpha-k)a}) - (2P/a) & -i(\alpha+k)(1-e^{-i(\alpha+k)a}) - (2P/a) \end{vmatrix} = 0.$$

This is readily multiplied out to give (11.21).