2.3.9. Alternate derivation of the Kronig-Penney equation[4]

First we recognize that the Schrödinger equation is of the form:

$$\frac{d^2\Psi}{dx^2} + U(x)\Psi = 0 \text{, where } U(x) = \frac{2m(V(x) - E)}{\hbar^2} \tag{2.3.41}$$

All solutions to this equation can be written as a linear combination of two arbitrary, but linearly independent, particular solutions. These can be chosen to be real since $U(x)$ is a real function.

Let the two particular solutions be $\Psi_1(x)$ and $\Psi_2(x)$. From the periodicity of $U(x)$:

$$U(x+a) = U(x) \tag{2.3.42}$$

it follows that $\Psi_1(x+a)$ and $\Psi_2(x+a)$ are also solutions, so that there exist real coefficients A_{11}, A_{12}, A_{21} and A_{22} for which:

$$\begin{bmatrix} \Psi_1(x+a) \\ \Psi_2(x+a) \end{bmatrix} = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \times \begin{bmatrix} \Psi_1(x) \\ \Psi_2(x) \end{bmatrix} \tag{2.3.43}$$

The solution for the actual wavefunction $\Psi(x)$ is a linear combination of the real solutions, $\Psi_1(x)$ and $\Psi_2(x)$, with coefficients p and q:

$$\Psi(x) = p\Psi_1(x) + q\Psi_2(x) \tag{2.3.44}$$

such that

$$\Psi(x+a) = \lambda\Psi(x) \tag{2.3.45}$$

This is an eigenvalue problem and a solution exists for,:

$$\begin{vmatrix} A_{11} - \lambda & A_{12} \\ A_{21} & A_{22} - \lambda \end{vmatrix} = 0 \tag{2.3.46}$$

The corresponding eigenvalues are:

$$\lambda_{1,2} = \frac{A_{11} + A_{22}}{2} \pm i\sqrt{(A_{11}A_{22} - A_{12}A_{21}) - (\frac{A_{11} + A_{22}}{2})^2} \tag{2.3.47}$$

[4] Courtesy of Willy Sierens, 10/02/2007

Since the wavefunction $\Psi(x)$ can also be expressed using Bloch functions:

$$\Psi(x) = u(x)\exp(\pm ikx) \text{ with } u(x+a) = u(x) \tag{2.3.48}$$

The eigenvalue equation can be reformulated as:

$$\Psi(x+a) = u(x)\exp(\pm ika)\exp(\pm ikx) = \Psi(x)\exp(\pm ika) \tag{2.3.49}$$

so that

$$\lambda_{1,2} = \exp(\pm ika) \tag{2.3.50}$$

Combining (2.3.47) with (2.3.50) results in:

$$A_{11} + A_{22} = \lambda_1 + \lambda_2 = 2\cos ka \tag{2.3.51}$$

We now construct the real functions $\Psi_1(x)$ and $\Psi_2(x)$ corresponding to the Kronig-Penney potential, while requiring the functions and their derivatives to be continuous at $x = 0$:

$$\begin{aligned} &\Psi_1(x) = \exp \alpha x \text{, for } -b < x < 0 \\ &\Psi_1(x) = \cos \beta x + \frac{\alpha}{\beta}\sin \beta x \text{, for } 0 < x < a\text{-}b \end{aligned} \tag{2.3.52}$$

and

$$\begin{aligned} &\Psi_2(x) = \exp(-\alpha x) \text{, for } -b < x < 0 \\ &\Psi_2(x) = \cos \beta x - \frac{\alpha}{\beta}\sin \beta x \text{, for } 0 < x < a\text{-}b \end{aligned} \tag{2.3.53}$$

where

$$\alpha = \frac{\sqrt{2m(V_0 - E)}}{\hbar} \text{ and } \beta = \frac{\sqrt{2mE}}{\hbar} \tag{2.3.54}$$

The wavefunctions in the section between $x = a\text{-}b$ and $x = a$, are now obtained using (2.3.43).

$$\begin{aligned} \Psi_1(x) = A_{11}\exp \alpha x + A_{12}\exp(-\alpha x) \text{, for } a\text{-}b < x < a \\ \Psi_2(x) = A_{21}\exp \alpha x + A_{22}\exp(-\alpha x) \text{, for } a\text{-}b < x < a \end{aligned} \tag{2.3.55}$$

Both functions and their derivatives also need to be continuous at $x = a\text{-}b$, leading to:

$$A_{11} = \frac{\alpha^2 - \beta^2}{2\alpha\beta}\exp \alpha b \sin \beta(a-b) + \exp \alpha b \cos \beta(a-b) \tag{2.3.56}$$

$$A_{22} = -\frac{\alpha^2 - \beta^2}{2\alpha\beta}\exp(-\alpha b)\sin\beta(a-b) + \exp(-\alpha b)\cos\beta(a-b) \qquad (2.3.57)$$

combining (2.3.56), (2.3.57) and (2.3.51) then yields:

$$\cos ka = \frac{\alpha^2 - \beta^2}{2\alpha\beta}\sinh\alpha b\sin\beta(a-b) + \cosh\alpha b\cos\beta(a-b) \qquad (2.3.58)$$