2.3.8. Derivation of the Kronig-Penney model

The solution to Schrödinger's equation for the Kronig-Penney potential previously shown in Figure 2.3.3 and discussed in section 2.3.2.1 is obtained by assuming that the solution is a Bloch function, namely a traveling wave solution of the form, e^{ikx}, multiplied with a periodic solution, $u(x)$, which has the same period as the periodic potential. The total wavefunction is therefore of the form:

$$\Psi(x) = u(x)e^{ikx} \qquad (2.3.18)$$

where $u(x)$ is the periodic function as defined by $u(x) = u(x + a)$, and $k(x)$ is the wave number. Rewriting the wavefunction in such form allows the simplification of the Schrödinger equation, which we now apply to region I, between the barriers where $V(x) = 0$ and region II, the barrier region where $V(x) = V_0$:

In region I, Schrödinger's equation becomes:

$$\frac{d^2u_I(x)}{dx^2} + 2ik\frac{du_I(x)}{dx} + (\beta^2 - k^2)u_I(x) = 0 \text{ for } 0 < x < a\text{-}b \qquad (2.3.19)$$

with

$$\beta = \frac{2\pi}{h}\sqrt{2mE} \qquad (2.3.20)$$

While in region II, it becomes:

$$\frac{d^2u_{II}(x)}{dx^2} + 2ik\frac{du_{II}(x)}{dx} - (k^2 + \alpha^2)u_{II}(x) = 0 \text{ for } a\text{-}b < x < a \qquad (2.3.21)$$

with

$$\alpha = \frac{2\pi}{h}\sqrt{2m(V_0 - E)} \qquad (2.3.22)$$

The solution to equations (2.3.6) and (2.3.8) are of the form:

$$u_I(x) = (A\cos\beta x + B\sin\beta x)e^{-ikx} \text{ for } 0 < x < a\text{-}b \qquad (2.3.23)$$

$$u_{II}(x) = (C\cosh\alpha x + D\sin\alpha x)e^{-ikx} \text{ for } a\text{-}b < x < a \qquad (2.3.24)$$

Since the potential, $V(x)$, is finite everywhere, the solutions for $u_I(x)$ and $u_{II}(x)$ must be continuous as well as their first derivatives. Continuity at $x = 0$ results in:

$$u_I(0) = u_{II}(0) \text{ so that } A = C \tag{2.3.25}$$

and continuity at $x = a\text{-}b$ combined with the requirement that $u(x)$ be periodic results in:

$$u_I(a-b) = u_{II}(-b) \tag{2.3.26}$$

so that

$$(A\cos\beta(a-b) + B\sin\beta(a-b))e^{-ik(a-b)} = (C\cosh\alpha b - D\sinh\alpha b)e^{ikb} \tag{2.3.27}$$

Continuity of the first derivative at $x = 0$ requires that:

$$\left.\frac{du_I(x)}{dx}\right|_{x=0} = \left.\frac{du_{II}(x)}{dx}\right|_{x=0} \tag{2.3.28}$$

The first derivatives of $u_I(x)$ and $u_{II}(x)$ are:

$$\frac{du_I(x)}{dx} = (A\beta\sin\beta x - B\beta\cos\beta x)e^{-ikx} - ik(A\cos\beta x + B\sin\beta x)e^{-ikx} \tag{2.3.29}$$

$$\frac{du_{II}(x)}{dx} = (C\alpha\sinh\alpha x + D\alpha\cosh\alpha x)e^{-ikx} - ik(C\cosh\alpha x + D\sinh\alpha x)e^{-ikx} \tag{2.3.30}$$

so that (2.3.15) becomes:

$$-B\beta - ikA = D\alpha - ikC \tag{2.3.31}$$

Finally, continuity of the first derivative at $x = a\text{-}b$, again combined with the requirement that $u(x)$ is periodic, results in:

$$\left.\frac{du_I(x)}{dx}\right|_{x=a-b} = \left.\frac{du_{II}(x)}{dx}\right|_{x=-b} \tag{2.3.32}$$

so that

$$\begin{aligned}
&(A\beta\sin\beta(a-b) - B\beta\cos\beta(a-b))e^{-ik(a-b)} \\
&- ik(A\cos\beta(a-b) + B\sin\beta(a-b))e^{-ik(a-b)} \\
&= (-C\alpha\sinh\alpha b + D\alpha\cosh\alpha b)e^{ikb} - ik(C\cosh\alpha b - D\sinh\alpha b)e^{ikb}
\end{aligned} \tag{2.3.33}$$

This equation can be simplified using equation (2.3.14) as:

$$(A\beta\sin\beta(a-b) - B\beta\cos\beta(a-b)) = (-C\alpha\sinh\alpha b + D\alpha\cosh\alpha b)e^{ika} \tag{2.3.34}$$

As a result we have four homogenous equations, (2.3.12), (2.3.14), (2.3.18), and (2.3.21), with four unknowns, *A*, *B*, *C*, and *D*, for which there will be a solution if the determinant of this set of equations is zero, or:

$$\begin{vmatrix} 1 & 0 & -1 & 0 \\ 0 & \beta & 0 & \alpha \\ \cos\beta(a-b) & \sin\beta(a-b) & -\cosh\alpha b \exp ika & \sinh\alpha b \exp ika \\ \beta\sin\beta(a-b) & -\beta\cos\beta(a-b) & \alpha\sin\alpha b\exp ika & -\alpha\cosh\alpha b \exp ika \end{vmatrix} = 0 \quad (2.3.35)$$

The first row of the determinant represents equation (2.3.12), the second row is obtained by combining (2.3.18) and (2.3.12), the third row represents equation (2.3.14) and the fourth row represents equation (2.3.21). This determinant can be rewritten as two determinants, each with three rows and column, while replacing $\cos\beta(a\text{-}b)$ by β_c, $\sin\beta(a\text{-}b)$ by β_s, $\cosh\alpha b\ e^{ika}$ by α_c and $\sinh\alpha b\ e^{ika}$ by α_s, which results in:

$$\begin{vmatrix} \beta & 0 & \alpha \\ \beta_s & -\alpha_c & \alpha_s \\ -\beta\beta_c & \alpha\alpha_s & -\alpha\alpha_c \end{vmatrix} = \begin{vmatrix} 0 & \beta & \alpha \\ \beta_c & \beta_s & \alpha_s \\ \beta\beta_s & -\beta\beta_c & -\alpha\alpha_c \end{vmatrix} \quad (2.3.36)$$

Working out the determinants and using $\beta_c^2 + \beta_s^2 = 1$, and $\alpha_c^2 - \alpha_s^2 = e^{2ika}$, one finds:

$$(\alpha^2 - \beta^2)\sinh\alpha b\sin\beta(a-b)\exp ika + 2\alpha\beta\cosh\alpha b\cos\beta(a-b)\exp ika = \alpha\beta(1+\exp 2ika) \quad (2.3.37)$$

And finally, substituting β_c, β_s, α_c and α_s:

$$\cos ka = F = \frac{\alpha^2 - \beta^2}{2\alpha\beta}\sinh\alpha b\sin\beta(a-b) + \cosh\alpha b\cos\beta(a-b) \quad (2.3.38)$$

where $e^{ika} + e^{-ika}$ was replaced by 2cos *ka*.

A further simplification is obtained as the barrier width, *b*, is reduced to zero while the barrier height, V_0, is increased to infinity in such manner that the product, bV_0, remains constant and the potential becomes a delta function train at $x = a$ and repeated with a period of *a*, namely $bV_0\delta(x - b - \text{n}a)$ where n is an integer. As *b* approaches zero, $\sinh\alpha b$ approaches αb. Equation (2.3.25) then reduces to:

$$\cos ka = F = P\frac{\sin\beta a}{\beta a} + \cos\beta a \quad (2.3.39)$$

with

$$\beta = \frac{\sqrt{2mE}}{\hbar} \text{ and } P = \frac{mV_0 ba}{\hbar^2} \quad (2.3.40)$$

