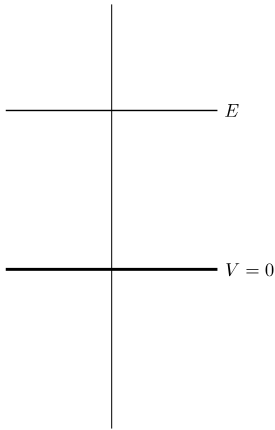# Kronig-Penney Model

by Dr. Colton, Physics 581 (last updated: Fall 2020)

First, two notes about the solution to the Schroedinger Equation for regions where the potential is constant.
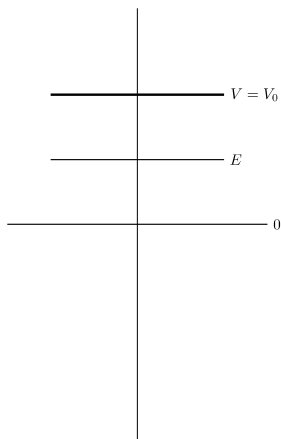
If the energy is higher than the potential, then the wavefunction is like

$$\psi = Ae^{iKx} + Be^{-iKx} \quad \text{(i.e. sines and cosines)}$$

where $K = \sqrt{\frac{2m}{\hbar^2}(E - V)} = \sqrt{\frac{2m}{\hbar^2}E}$ (since $V = 0$ for this section, in this example)

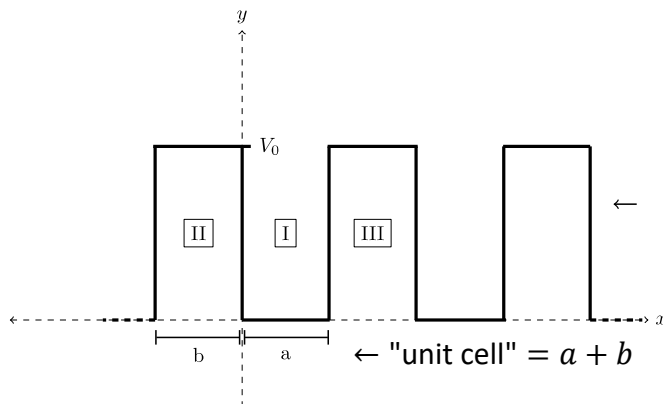K has units of rad/m but it is a measure of energy.

If the potential is higher than the energy, then the wavefunction is like

$$\psi = Ce^{Qx} + De^{-Qx} \quad \text{(i.e. real exponentials)}$$

where $Q = \sqrt{\frac{2m}{\hbar^2}(V_0 - E)}$

Q has units of rad/m but is a measure of $V_0 - E$, i.e. how far below the potential the energy is.

Kronig-Penney Potential

← Look for bound states, they will have energy around here.

← "unit cell" $= a + b$

Region I: $\Psi_I = Ae^{iKx} + Be^{-iKx}$
Region II: $\Psi_{II} = Ce^{iQx} + De^{-iQx}$
Region III: Connected to Ψ_{II} via Bloch's Theorem
$$\Psi_{III} = e^{ik(a+b)}\Psi_{II}$$

Kronig-Penney model – pg 1

Boundary conditions: ψ must be continuous, and also ψ' must be continuous. Apply to each of the two boundaries.

Boundary between II and I, at $x = 0$

   1) $\psi_{II}(x = 0) = \psi_I(x = 0)$
$$Ce^0 + De^0 = Ae^0 + Be^0 \rightarrow \underline{A + B = C + D}$$

   2) $\psi_{II}'(x = 0) = \psi_I'(x = 0)$
$$QC - QD = iKA - iKB \rightarrow \underline{iK(A - B) = Q(C - D)}$$

Boundary between I and III, at $x = a$

   3) $\psi_I(x = a) = \psi_{III}(x = a) = e^{ik(a+b)}\psi_{II}(x = -b)$
$$\underline{Ae^{iKa} + Be^{-iKa} = e^{ik(a+b)}[Ce^{-Qb} + De^{Qb}]}$$

   4) $\psi_I'(x = a) = \psi_{III}'(x = a) = e^{ik(a+b)}\psi_{II}'(x = -b)$
$$\underline{AiKe^{iKa} - BiKe^{-iKa} = e^{ik(a+b)}[CQe^{-Qb} - DQe^{Qb}]}$$

Write the four underlined equations as a single matrix equation

$$0 = \begin{pmatrix} & & & \\ & M & & \\ & & & \\ & & & \end{pmatrix} \begin{pmatrix} A \\ B \\ C \\ D \end{pmatrix}$$
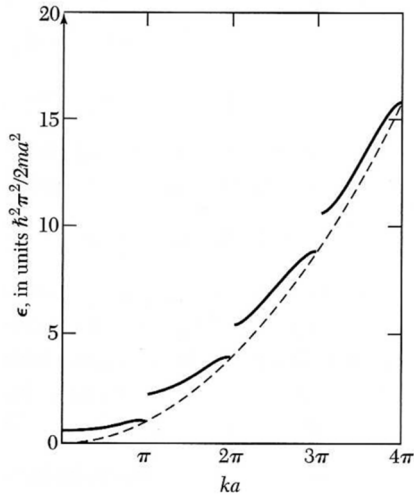
E.g. the first row comes from $A + B = C + D \rightarrow 0 = -A - B + C + D$, so the first row of the matrix M is $(-1, -1, +1, +1)$.

To solve, set $\det(M) = 0$. Textbook: "It is rather tedious to obtain this [next] equation…"

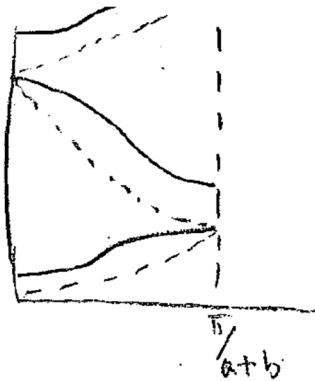$$\boxed{\frac{Q^2 - K^2}{2QK}\sinh(Qb)\sin(Ka) + \cosh(Qb)\cos(Ka) = \cos[k(a + b)]}$$

Q and K have E in them, so in principle, given a k we can solve for E to get $E(k)$! In practice must be done numerically.

Result:

Kittel Fig 7.6, pg 170. Plot of energy vs. wavenumber for the Kronig-Penney potential for a certain choice of V_0, a, and b. Notice the energy gaps at $ka = \pi, 2\pi, 3\pi, ...$

Or, if you translate back to the first BZ, it looks like this:

Kittel Fig 7.6, pg 170, translated back to the first BZ.

Disclaimer: these plots are not <u>really</u> of the boxed equation above. They are plots of the situation where $b \to 0$, $V_0 \to \infty$, and $b \cdot V_0 = \text{constant} = \dfrac{3\pi}{2} \dfrac{\hbar^2}{ma}$ (Dirac delta function potential)

This limit gives rise to this variation of the equation,

$$\boxed{\left(\frac{P}{Ka}\right)\sin(Ka) + \cos(Ka) = \cos(ka)}$$

This is what is plotted in Kittel Fig 7.6 with, $P = \dfrac{3\pi}{2}$.

<u>Appendix:</u> Proof that second boxed equation is the limiting case of first boxed equation

1) $\cos k(a + b) \rightarrow \cos a$ since $b \rightarrow 0$
2) Observe that $Q \gg K$ (because Q contains a V_0 in it)

   So $\dfrac{Q^2-K^2}{2QK} \rightarrow \dfrac{Q}{2K}$

3) $Qb \rightarrow \left(\sqrt{\dfrac{2m(V_0-E)}{\hbar^2}} \right) b = \sqrt{\dfrac{2mV_0}{\hbar^2}} \, b = \sqrt{\dfrac{2m}{\hbar^2} \underbrace{(bV_0)}_{\text{constant}} \cdot \underbrace{b}_{\text{small}}}$

   Therefore,

$$\sinh(Qb) \approx Qb$$
$$\cosh(Qb) \approx 1$$

   First boxed equation becomes:

$$\frac{Q}{2K}(Qb) \sin Ka + (1) \cos Ka = \cos ka$$

   or

$$\frac{P}{Ka} \sin Ka + \cos Ka = \cos ka, \quad \text{with} P = \frac{Q^2 ba}{2}$$