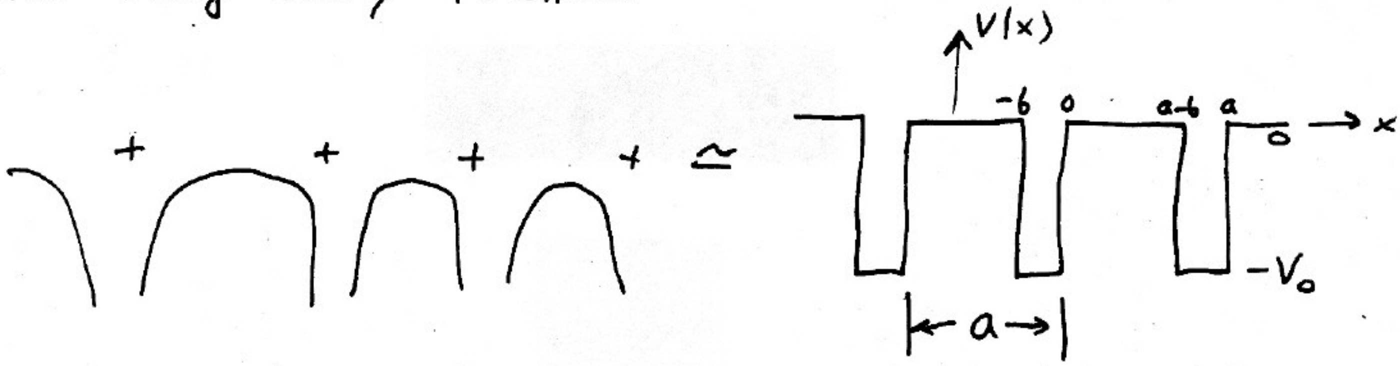
Solve a Real 1D Periodic Potential Schröd Equation.

The Kronig-Penney Potential



Wells of depth $-V_0$, of width b, spaced a apart.

$$V(x) = \begin{cases} 0 & 0 < x < a-b \\ -V_0 & -b < x < 0 \\ V(x+a) & \text{for all } x. \end{cases}$$

The 1D Schröd. Eq. is:

$$\frac{d^2u}{dx^2} + \frac{2mE}{\hbar^2}u = 0 \qquad 0 < x < a-b$$

$$\frac{d^2u}{dx^2} + \frac{2m(E+V_0)}{\hbar^2}u = 0 \qquad -b < x < 0$$

These have the form   Looking for solutions with $E > 0$.

$$u'' = -k^2 u \quad \Rightarrow \quad u \sim e^{ikx}, e^{-ikx}$$

$$u(x) = \begin{cases} Ae^{i\alpha x} + Be^{-i\alpha x} & 0 < x < a-b \\ Ce^{i\beta x} + De^{-i\beta x} & -b < x < 0 \end{cases} \qquad \alpha = \sqrt{\frac{2mE}{\hbar^2}} \qquad \beta = \sqrt{\frac{2m(E+V_0)}{\hbar^2}}$$

Now apply the BC's

(I) At $x=0$ $u(x)$ and $\frac{du}{dx}$ are continuous

$x=0$

$$Ae^{i0}+Be^{i0} = Ce^{i0}+De^{i0}$$

or $\boxed{A+B=C+D}$

and $\boxed{i\alpha A - i\alpha B = i\beta C - i\beta D}$ from continuity of du/dx.

(II) We expect the solutions to be of the Bloch type:

$$u(x) = e^{ikx}\phi(x)$$ where k is some wavevector

where $$\phi(x+a) = \phi(x)$$

So multiply $u(x)$ by e^{-ikx} and make that thing periodic in x with period a.

i.e. $e^{-ikx}u(x)$

$$\phi(x) = \begin{cases} Ae^{i(\alpha-k)x} + Be^{-i(\alpha+k)x} & 0<x<a-b \\ Ce^{i(\beta-k)x} + De^{-i(\beta+k)x} & -b<x<0 \end{cases}$$

For instance

$$\phi(-b) = \phi(a-b)$$

and

$$\left.\frac{d\phi}{dx}\right|_{x=-b} = \left.\frac{d\phi}{dx}\right|_{x=a-b}$$

Momentary diversion on the subject of periodic potentials...

An equation of the form:

$$\frac{d^2y}{dx^2} + f(x)\,y = 0$$

where $f(x)$ is an <u>even</u> <u>periodic</u> function, is known as a HILL EQUATION

$f(-x) = f(x)$

$f(x+a) = f(x)$

In particular, a Mathieu Diff. Eq. has the form

$$\frac{d^2y}{dx^2} + (\alpha + \beta\cos 2x)\,y = 0 \qquad \alpha, \beta \text{ constants}$$

Like a periodic $V(x)$

Floquet's Thm says that you can always find a solution to Mathieu's Eq. of the form:

$$y(x) = e^{\mu x}\,\phi(x)$$

where $\phi(x)$ is periodic

These equations result in

$$\boxed{A\, e^{i(\alpha-h)(a-b)} + B e^{-i(\alpha+h)(a-b)} = C e^{-i(\beta-h)b} + D e^{+i(\beta+h)b}}$$

and,

$$\boxed{i(\alpha-h) A e^{i(\alpha-h)(a-b)} - i(\alpha+h) B e^{-i(\alpha+h)(a-b)} = i(\beta-h) C e^{-i(\beta-h)b} - i(\beta+h) D e^{i(\beta+h)b}}$$

We now have 4 linear and independent equations for A, B, C, D.
This problem can be solved with linear algebra

$$\begin{pmatrix} 1 & 1 & -1 & -1 \\ i\alpha & -i\alpha & -i\beta & i\beta \\ e^{i(\alpha-h)(a-b)} & e^{-i(\alpha+h)(a-b)} & -e^{-i(\beta-h)b} & -e^{i(\beta+h)b} \\ i(\alpha-h)e^{i(\alpha-h)(a-b)} & -i(\alpha+h)e^{-i(\alpha+h)(a-b)} & -i(\beta-h)e^{-i(\beta-h)b} & i(\beta+h)e^{i(\beta+h)b} \end{pmatrix} \begin{pmatrix} A \\ B \\ C \\ D \end{pmatrix} = 0$$

$$\bar{\bar{M}}\, \vec{V} = 0$$

Set

$$\det(\bar{\bar{M}}) = 0$$

~~and solve for to get the answer.~~

"After considerable algebra, this reduces to"

$$\frac{-\beta^2-\alpha^2}{2\alpha\beta}\sin\beta b\,\sin[\alpha(a-b)] + \cos\beta b\,\cos[\alpha(a-b)] = \cos ha$$

This can be simplified if we consider the wells to be very narrow and very deep:

$$b \to 0$$
$$V_0 \to \infty$$

such that

$$\beta^2 b \sim b\,V_0 \quad \text{remains finite}$$

so

$$\beta b \sim b\sqrt{V_0} \to 0$$

and

$$\sin(\beta b) \simeq \beta b$$
$$\cos(\beta b) \simeq 1$$
$$a-b \simeq a$$

Then

$$-\frac{(\beta^2+\alpha^2)}{2\alpha\cancel{\beta}}\beta b\,\sin(\alpha a) + \cos(\alpha a) = \cos ha$$

or $$-\frac{\beta^2 b}{2\alpha}\sin(\alpha a) + \cos(\alpha a) = \cos(ha)$$

~~Let~~ $\cancel{P = \frac{\beta^2 b}{2\alpha}}$

or

$$-\frac{\beta^2 ba}{2}\frac{\sin(\alpha a)}{(\alpha a)} + \cos(\alpha a) = \cos(ha)$$

Define $$P \equiv \frac{\beta^2 b a}{2}$$

This is a dimensionless number which characterizes the strength of the periodic part of the potential

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If $P = 0$ (no periodic part of the potential)
then

$$\cos(\alpha a) = \cos(ka)$$

or

$$\alpha = k = \sqrt{\frac{2mE}{\hbar^2}} \Rightarrow E = \frac{\hbar^2 k^2}{2m}$$

Free particle!

$\cos(ka)$ is bounded between -1 and $+1$.

$$-P\frac{\sin(\alpha a)}{\alpha a} + \cos(\alpha a) = \cos(ka)$$

When the LHS exceeds ± 1, there is no solution for any k. This leads to an energy gap.

Note that the gaps appear near $ka = \pi, 2\pi$, etc,

or $$k = \frac{\pi}{a}, \frac{2\pi}{a}, \ldots$$

Just as we saw in the Bragg refraction case.

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In[32]:= Plot[ {lhs[αa, 10], 1, -1}, {αa, 0, 20}, PlotRange → {-3, 3}, PlotPoints → 500]
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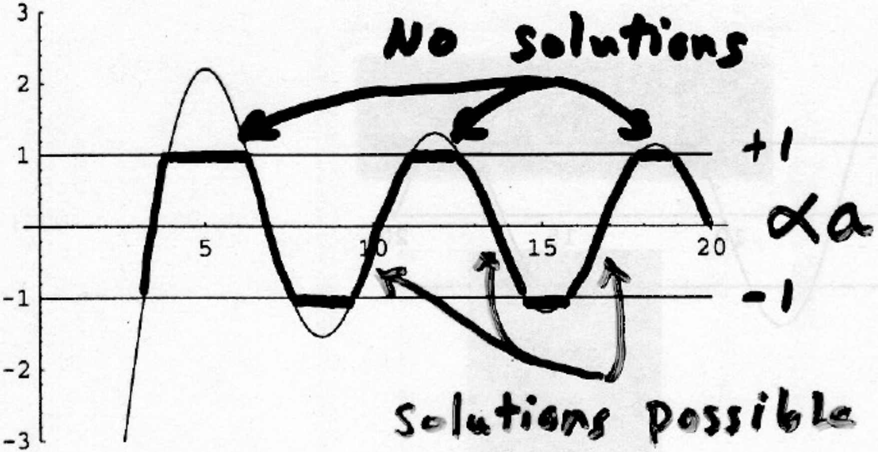


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Out[32]= - Graphics -
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