Kronig-Penney Model:

(not on exam 1)

(application to Solid State Physics)

$$V(x) = \frac{\hbar^2}{2m} \frac{\lambda}{a} \sum_{n=-\infty}^{\infty} \delta(x - na)$$

Let $\psi(x) = A_n \sin k(x-na) + B_n \cos k(x-na)$
for $(n-1)a \le x \le na$.

The boundary conditions at $x = n$ are:

$$\psi(na) = B_n = A_{n+1} \sin k(-ka) + B_{n+1} \cos k(- a)$$

$$\begin{aligned}\psi'(na^+) - \psi'(na^-) &= A_{n+1} k \cos(-ka) + B_{n+1}(-k) \sin k(- a) \\ &\quad - A_n k \\ &= \frac{\lambda}{a} \psi(na) = \frac{\lambda}{a} B_n .\end{aligned}$$

$$\rightarrow \quad \begin{aligned} -A_{n+1} \sin(ka) + B_{n+1} \cos(ka) &= B_n \\ A_{n+1} \cos(ka) + B_{n+1} \sin(ka) &= A_n + \frac{\lambda}{ka} B_n \end{aligned}$$

Let $g = \lambda/ka$.

$$\begin{pmatrix} -\sin(ka) & \cos(ka) \\ \cos(ka) & \sin(ka) \end{pmatrix} \begin{pmatrix} A_{n+1} \\ B_{n+1} \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 1 & g \end{pmatrix} \begin{pmatrix} A_n \\ B_n \end{pmatrix}$$

$$\begin{pmatrix} A_{n+1} \\ B_{n+1} \end{pmatrix} = \begin{pmatrix} -\sin(ka) & \cos(ka) \\ \cos(ka) & \sin(ka) \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & g \end{pmatrix} \begin{pmatrix} A_n \\ B_n \end{pmatrix}$$

$$= \underbrace{\begin{pmatrix} \cos(ka) & -\sin(ka) + g\cos(ka) \\ \sin(ka) & \cos(ka) + g\sin(ka) \end{pmatrix}}_{M} \begin{pmatrix} A_n \\ B_n \end{pmatrix}$$

Since this is true for any n,

$$\begin{pmatrix} A_{n+1} \\ B_{n+1} \end{pmatrix} = M \begin{pmatrix} A_n \\ B_n \end{pmatrix}, \quad \begin{pmatrix} A_{n+2} \\ A_{n+2} \end{pmatrix} = M \begin{pmatrix} A_{n+1} \\ B_{n+1} \end{pmatrix}$$

$$\rightarrow \begin{pmatrix} A_{n+2} \\ B_{n+2} \end{pmatrix} = M^2 \begin{pmatrix} A_n \\ B_n \end{pmatrix} \text{ and in general,}$$

$$\begin{pmatrix} A_{n+m} \\ B_{n+m} \end{pmatrix} = M^m \begin{pmatrix} A_n \\ B_n \end{pmatrix} \text{ and } \begin{pmatrix} A_n \\ B_n \end{pmatrix} = M^{-m} \begin{pmatrix} A_{n+m} \\ B_{n+m} \end{pmatrix}.$$

On physical grounds we do not want $\begin{pmatrix} A_n \\ B_n \end{pmatrix}$ to diverges as $n \rightarrow \infty$ or as $n \rightarrow -\infty$. The wavefunction would not be normalizable if it did diverge.

Determine the eigenvalues of M:

$$M \underbrace{\begin{pmatrix} C_1 \\ C_2 \end{pmatrix}}_{\text{eigenvector}} = \underbrace{\Lambda}_{\text{eigenvalue}} \begin{pmatrix} C_1 \\ C_2 \end{pmatrix}$$

$$\rightarrow (M - \Lambda \mathbb{1}) \begin{pmatrix} C_1 \\ C_2 \end{pmatrix} = 0 \quad \longrightarrow \quad \det(M - \Lambda \mathbb{1}) = 0.$$

$$\begin{Vmatrix} \cos(ka) - \Lambda & -\sin(ka) + g\cos(ka) \\ \sin(ka) & \cos(ka) + g\sin(ka) - \Lambda \end{Vmatrix} =$$

$$= \cos^2(ka) + g\sin(ka)\cos(ka) - \Lambda(2\cos(ka) + g\sin(ka)) + \Lambda^2 + \sin^2(ka) - g\sin(ka)\cos(ka)$$

$$\rightarrow 0 = \Lambda^2 - \Lambda(2\cos(ka) + g\sin(ka)) + 1$$

$$\rightarrow \Lambda = \frac{2\cos(ka) + g\sin(ka) \pm \sqrt{(2\cos(ka) + g\sin(ka))^2 - 4}}{2}$$

Let $\alpha = \cos(ka) + \frac{g}{2}\sin(ka)$.

Then $\Lambda = \alpha \pm \sqrt{\alpha^2 - 1}$.

<u>Case 1:</u> $|\alpha| < 1$, $\Lambda = \alpha \pm i\sqrt{1-\alpha^2}$, $|\ \ | = 1$

<u>Case 2:</u> $|\alpha| = 1$, $\Lambda = \alpha$, $|\ \ | = 1$

<u>Case 3:</u> $|\alpha| > 1$, $\Lambda = \alpha \pm \sqrt{\alpha^2 - 1}$,

Since $|\alpha| > \sqrt{\alpha^2-1}$, one eigenvalue has $|\Lambda| > 1$ and one has $|\Lambda| < 1$.

Case 3 is not physical since $\begin{pmatrix} A_n \\ B_n \end{pmatrix}$ will diverge as either $n \to \infty$ or $n \to -\infty$:

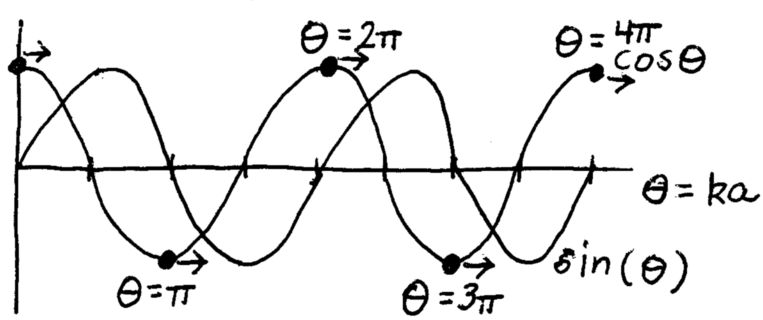
$$M^m \begin{pmatrix} C_1 \\ C_2 \end{pmatrix} = \Lambda^m \begin{pmatrix} C_1 \\ C_2 \end{pmatrix}.$$

Remembering that $g = \frac{\lambda}{ka}$, if we plot

$\alpha = \cos(ka) + \frac{g}{2(ka)} \sin(ka)$ vs. k, there will

only be solutions for $|\alpha| \leq 1$.

As shown on the following page, there are gaps near $ka = n\pi$. At these points $\cos(ka) = \pm 1$, and sin is changing sign - so the magnitude of α must be bigger than 1 either for $ka > n\pi$ or $ka < n\pi$.

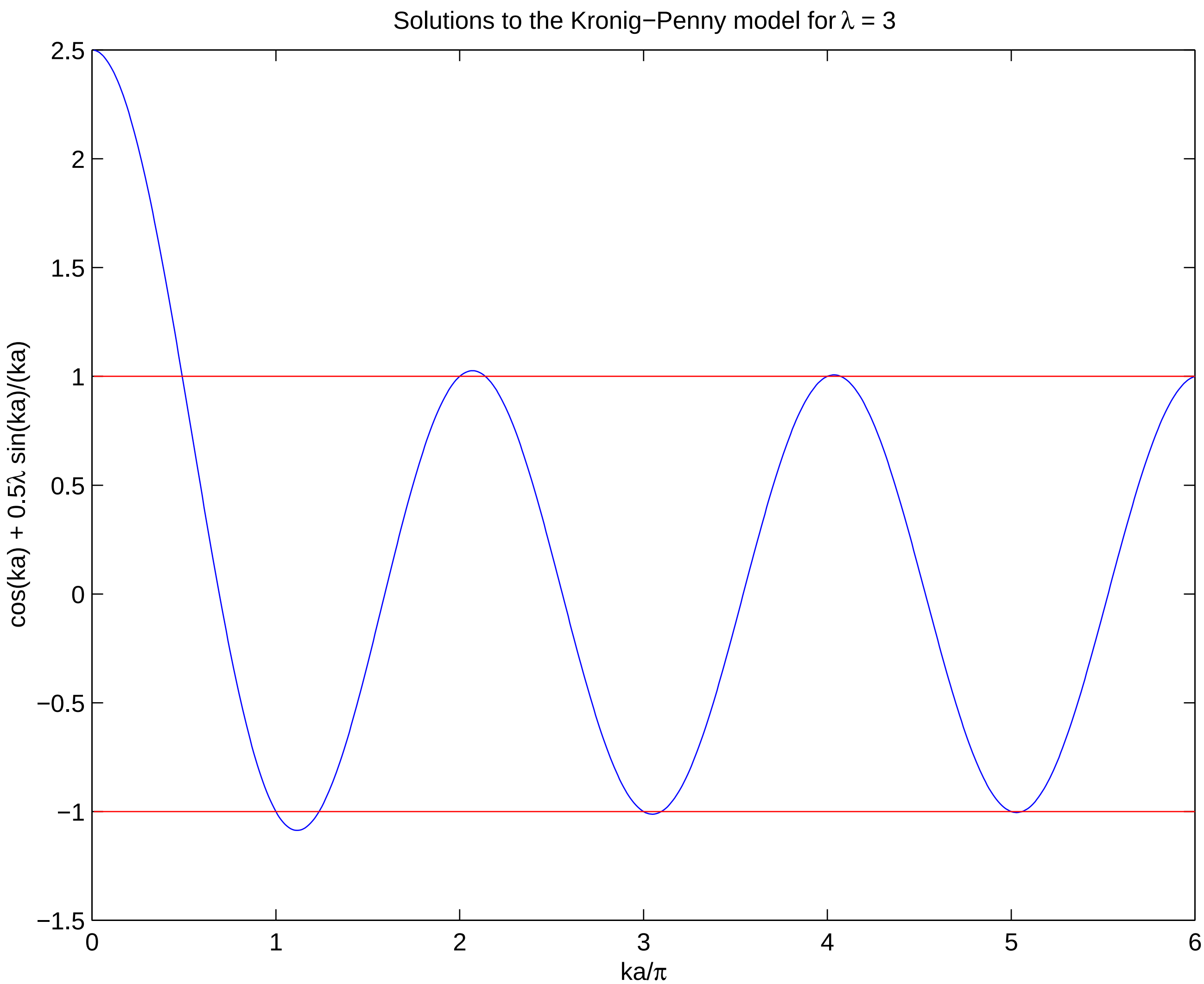


Note the gap occur to the right of $\theta = n\pi$ (see arrows).

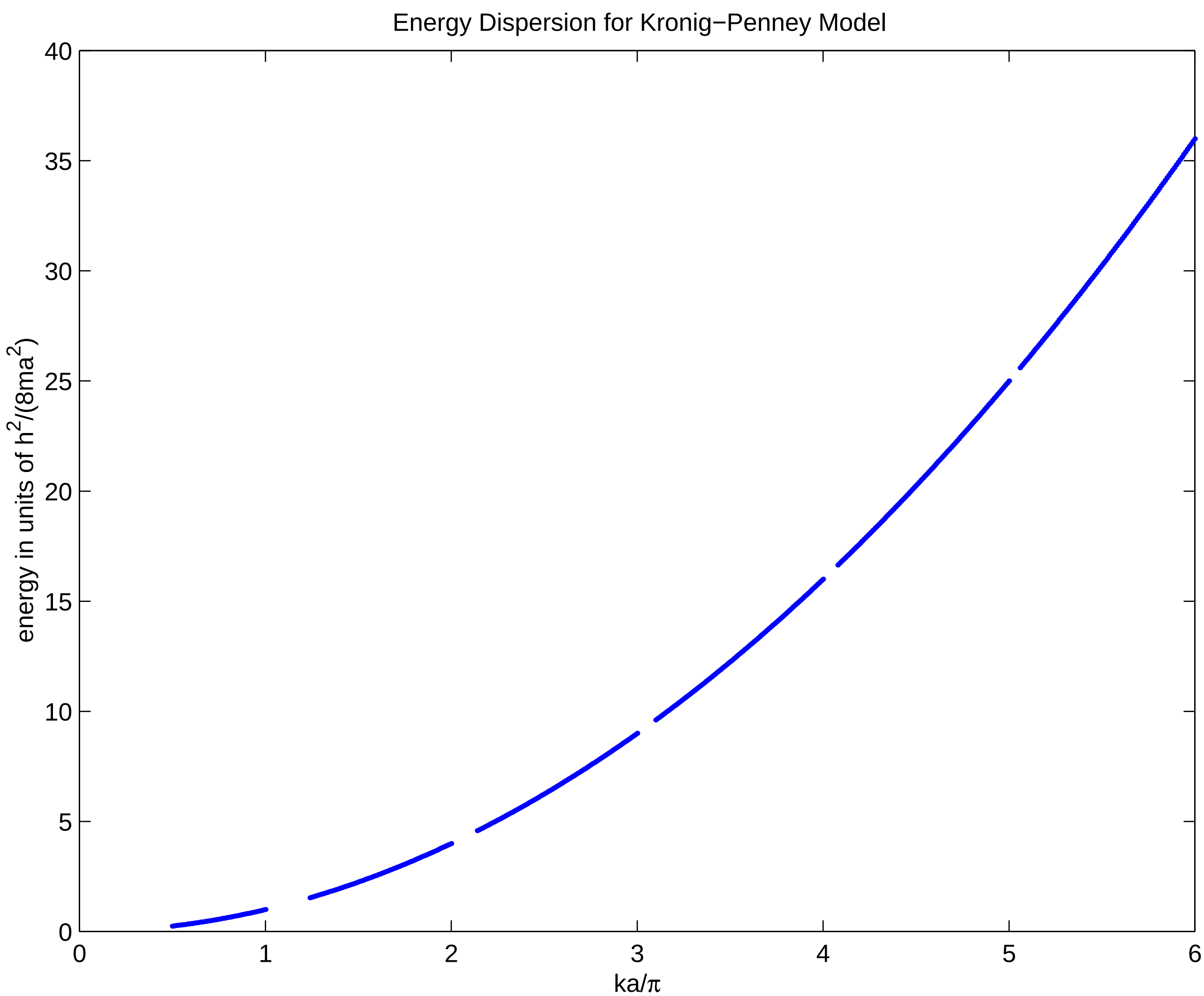
What is the significance?

In a periodic potential there are gaps or regions of forbidden energy. The regions between the gaps are called bands.

When you fill up the states in a solid w/electrons, if the you just fill a band up, then the next empty state will require an energy E_g. If $E_g >> k_B T$, you will get an insulator.



Solutions to the Kronig−Penny model for λ = 3
2.5
2
1.5
1
0.5
0
−0.5
−1
−1.5
0
1
2
3
4
5
6
ka/π
cos(ka) + 0.5λ sin(ka)/(ka)


Energy Dispersion for Kronig−Penney Model
energy in units of h²/(8ma²)
ka/π
0
5
10
15
20
25
30
35
40
0
1
2
3
4
5
6