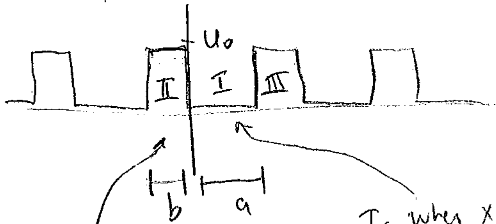
~~[illegible]~~ Jly 28 pg 1

Kronig - Penney Model



← energy here, otherwise unbound situation.
Want E vs k, like ball + springs model for phonons

I. when x in here, $V=0$

Solns are e^{+iKx} and e^{-iKx} → oscillations

See next page

ψ = linear combination

$\psi_I = A e^{iKx} + B e^{-iKx}$ and $E = \frac{\hbar^2 K^2}{2m}$

II. in here

$\psi_{II} = C e^{Qx} + D e^{-Qx}$ (because $U > E$) and $U_0 - E = \frac{\hbar^2 Q^2}{2m}$

exp. decay

a bit weird, but mathematically OK

check! ✓

* lower case k, now refers to Bloch thm.

III Bloch theorem: $\psi_{III} = e^{ik(a+b)} \psi_{II}$

(n = 1 because it's next unit cell over)

Bndy cond between II and I at $x=0$: (1) $\psi_{II}(x=0) = \psi_I(x=0)$

$C e^0 + D e^0 = A e^0 + B e^0 \rightarrow \boxed{A + B = C + D}$

(2) $\psi'_{II}(x=0) = \psi'_I(x=0)$

$QC - QD = iKA - iKB \longrightarrow \boxed{iK(A-B) = Q(C-D)}$

Bndy between I and III at $x = a$: (1) $\psi_I(x=a) = \psi_{III}(x=a) = e^{ik(a+b)} \psi_{II}(x=-b)$

$= e^{ik(a+b)} \cdot \psi_{II}\big|_{x=-b}$

$\boxed{A e^{iKa} + B e^{-iKa} = e^{ik(a+b)} \left[C e^{-Qb} + D e^{+Qb} \right]}$

(2) $\psi'_I(x=a) = \psi'_{III}(x=a) = e^{ik(a+b)} \psi'_{II}(x=-b)$

$\boxed{AiK e^{iKa} - BiK e^{-iKa} = e^{ik(a+b)} \left[+CQ e^{-Qb} - DQ e^{+Qb} \right]}$

Check of (2)

$AiK e^{iKx} - BiK e^{-iKx}\big|_{x=a}$

$= e^{ik(a+b)} \left[CQ e^{Qx} - DQ e^{-Qx} \right]\big|_{x=-b}$

$AiK e^{-iKb} - BiK e^{+iKb}$

$= e^{ik(a+b)} \left[CQ e^{-Qb} - DQ e^{Qb} \right]$

Kittel correct ✓

$$0 = \left(\quad M \quad \right) \begin{pmatrix} A \\ B \\ C \\ D \end{pmatrix}$$

check [illegible] Kittel has C and $-D$ p. 169

Proof that functions have the form given for the two types of regions

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi = E\psi$$

if V = constant:

$V <$ energy, then

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = +(E-V)\psi$$

$$\frac{d^2\psi}{dx^2} = \left(-\frac{2m}{\hbar^2}(E-V)\right)\psi$$ a negative number

solns: $\psi = C_1 \cos\left[\left(\sqrt{\frac{2m}{\hbar^2}(E-V)}\right)x\right]$
or $C_2 \sin\left[\left(\sqrt{\frac{2m}{\hbar^2}(E-V)}\right)x\right]$ } an independent pair

or $C_3 e^{i(\quad)x}$
or $C_4 e^{-i(\quad)x}$ } an independent pair

$V >$ energy then

...

$$\frac{d^2\psi}{dx^2} = \left(+\frac{2m}{\hbar^2}(V-E)\right)\psi$$ a positive number

the above solns don't work! (Try one)

solns: $\psi = C_1 e^{\sqrt{\frac{2m}{\hbar^2}(V-E)}\,x}$
or $\psi = C_2 e^{-\sqrt{\frac{2m}{\hbar^2}(V-E)}\,x}$ } an independent pair

Kronig-Penney cont.

Nontrivial solns → det M = 0

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

Kittel.. "It is rather tedious to obtain this equation"

Recall: $Q = \sqrt{\frac{2m(U_0-E)}{\hbar^2}}$

$K = \sqrt{\frac{2m(E-0)}{\hbar^2}} = \sqrt{\frac{2mE}{\hbar^2}}$

Could visualize solving for E in terms of k. Answer:

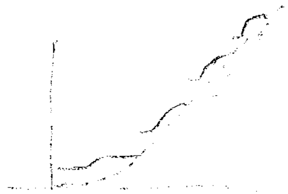
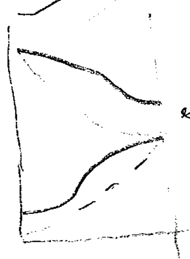


Fig 6 pg 170

in reduced BZ picture



← band gaps!

OK, not really the answer for all a+b ... to make the plot, he took limit as $\boxed{b \to 0}$ and $\boxed{U_0 \to \infty}$, basically keeping $\boxed{bU_0 = \text{constant}}$ (Dirac delta function)

To be precise For graph, $\frac{Q^2ba}{2} = \frac{3\pi}{2} = "P"$

$\left(\frac{m}{\hbar^2}(U_0-E)\right)ba = \frac{3\pi}{2}$

$(U_0-E)b = \text{constant} = \frac{3\pi}{2}\frac{\hbar^2}{ma}$

$U_0 b = \text{constant}$ $\quad U_0 b = \frac{3\pi}{2}\frac{\hbar^2}{ma} + E\overset{\to 0}{b}$

~~(if E = constant)~~

since $E \ll U_0$ which is true w/ delta function

For general P, the eqn becomes

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

proof on next page

but plotted for $P = \frac{3\pi}{2}$

Exam or HW: • show bottom eqn results with that approximation from top eqn

• show that the graph results from bottom eqn when $P = \frac{3}{2}\pi$. other values?

• graph top eqn w/o the delta function approx?

plot in reduced zone?

Proof that 1st Kronig Penney Eqn = 2nd Kronig Penney Eqn.

Can skip

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

little k

$$Q = \sqrt{\frac{2m(U_0-E)}{\hbar^2}}$$

$$K = \sqrt{\frac{2mE}{\hbar^2}}$$

Limit as $b \to 0$ RHS = $\cos(ka)$

Limit as $U_0 \to \infty$ then $Q \gg K$ $\frac{Q^2-K^2}{2QK} = \frac{Q^2}{2QK} = \frac{Q}{2K}$

Keep bU_0 = constant $Qb = \left(\sqrt{\frac{2m(U_0-E)}{\hbar^2}}\right) b$

$$= \sqrt{\frac{2mU_0}{\hbar^2}}\; b$$

$$= \sqrt{\frac{2m}{\hbar^2} b^2 U_0}$$

$$= \sqrt{\frac{2m}{\hbar^2} \underset{\text{constant}}{(bU_0)} \cdot \underset{\text{small!}}{b}}$$

$$Qb \ll 1$$

Small "angle": $\sinh x \simeq \frac{e^x - e^{-x}}{2} = \frac{\cancel{1}+x-(\cancel{1}-x)}{2} = x$

$$\cosh x \simeq \frac{e^x+e^{-x}}{2} = \frac{1+\cancel{x}+1-\cancel{x}}{2} = 1$$

Eqn becomes

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

Let $P = \frac{Q^2 ba}{2} \rightarrow \frac{Q^2 b}{2} = \frac{P}{a}$

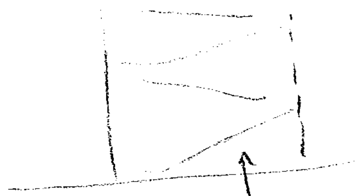
$$\boxed{\frac{P}{Ka}\sin Ka + \cos Ka = \cos ka}$$

How to determine where Fermi level is

Example w/ Si band structure (handout)

Si = diamond structure → 2 atoms / prim. cell

4 valence electrons / atom → 8 electrons / prim. cell

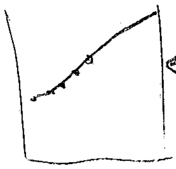


each band fills up with 2N electrons (including spin)

∴ $\boxed{\text{lowest 4 bands = filled}}$

(carefull w/ degenerate bands, though)

Metals vs insulators - where is Fermi Energy?



← if E_F here, metal

← Example: sodium metal, valency = 1

bcc → 1 atom/primitive unit cell

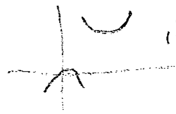
∴ $\frac{1}{2}$ band fills up

(2 spins per state)

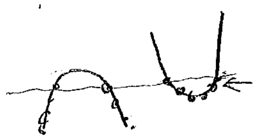
← if E_F here, insulator

(or semiconductor, if $E_g \lesssim 3$ eV)

direct gap vs



indirect gap



← E_F

semimetal

Ex: Bismuth, arsenic, antimony

Not many states for electrons to jump into.

~~Perturbation theory handout~~
~~(Nearly Free Electron)~~
~~- covered steps 1, 2, 3 today~~