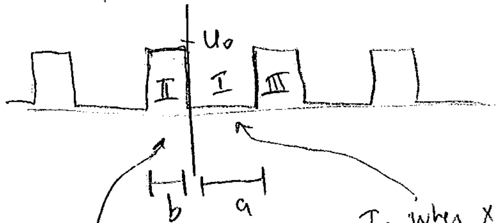
(Day 26 guest lecture) day 27 pg 1

Kronig - Penney Model



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

See next page

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

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

ψ = linear combination

$\psi_I = Ae^{iKx} + Be^{-iKx}$ and $E = \frac{\hbar^2 K^2}{2m}$

II. in here

$\psi_{II} = Ce^{Qx} + De^{-Qx}$ (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) $\psi_{II}(x=0) = \psi_I(x=0)$

$Ce^0 + De^0 = Ae^0 + Be^0 \rightarrow \boxed{A+B = C+D}$

(2) $\psi_{II}'(x=0) = \psi_I'(x=0)$

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

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

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

$\boxed{Ae^{iKa} + Be^{-iKa} = e^{ik(a+b)}\left[Ce^{-Qb} + De^{+Qb}\right]}$

(2) $\psi_I'(x=a) = \psi_{III}'(x=a) = e^{ik(a+b)}\psi_{II}'(x=-b)$

$\boxed{AiKe^{iKa} - BiKe^{-iKa} = e^{ik(a+b)}\left[+CQe^{-Qb} - DQe^{+Qb}\right]}$

Check of (2)

$AiKe^{iKx} - BiKe^{-iKx}\Big|_{x=a}$

$= e^{ik(a+b)}\left[CQe^{Qx} - DQe^{-Qx}\right]\Big|_{x=-b}$

$AiKe^{iKa} - BiKe^{-iKa}$

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

Kittel correct ✓

$$0 = \begin{pmatrix} & & \\ & M & \\ & & \end{pmatrix}\begin{pmatrix} A \\ B \\ C \\ D \end{pmatrix}$$

~~check wikipedia ... has ... pg 4 of 4~~

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

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

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

...

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

Non trivial 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 ... took limit as $b \to 0$ and $U_0 \to \infty$, basically keeping $b \cdot U_0$ = constant (Dirac delta function)

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

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

$(U_0 - E) b$ = constant

$U_0 b$ = constant

(~~if E = constant~~)

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

then eqn becomes

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

Exam or HW: • show bottom eqn results with that approximation from top eqn
• show that the graph results from bottom eqn when $P = \frac{3\pi}{2}$. other values? plot in reduced zone?
• graph top eqn w/o the delta function approx?