How to use Central Eqn.

1) Calculate Fourier coeffs of U

2) Pick a particular k value you're interested in

3) Truncate the Fourier expansion of U to some appropriate level (perhaps 2-4 coefficients) $\Rightarrow$ a set of G's and U_G's

4) Figure out which k's are connected to your particular k via those G's.

5) Write down eqns for each of the k's:
   your k plus the connected k's.
   There are a lot of C_k's in the eqns
   (and C_{k-G}, which is C_k for a different k)

6) Throw out all C_k's that don't match any of your set of k's.

7) You are left with say 5 equations and 5 unknowns
   (C_k's for your k + connected k's)

8) Solve matrix eqn!
   gives you say 5 different E values for that k
   (the values for first 5 bands)

Compare w/ calculating Madelung constant: do a summation, cut off at a certain point in real space
say farther distances don't matter

Here: cut summation off at a certain point in <u>reciprocal</u> space
say farther spatial frequencies don't matter.

Example: Hows the Central Eqn might be used. (from Peter Yu's final exam)

- GaAs crystal, assume only waves which couple to a given state are those with V_G components for $|G| < 4\pi/a$. Set up equations

Soln: GaAs is fcc lattice

$$\vec{G} = h\vec{b_1} + k\vec{b_2} + l\vec{b_3}$$

look up $\vec{b_1}, \vec{b_2}, \vec{b_3}$ in Ch. 2

$$\left.\begin{aligned} \vec{b_1} &= 2\pi/a\ (-1,1,1) \\ \vec{b_2} &= 2\pi/a\ (1,-1,1) \\ \vec{b_3} &= 2\pi/a\ (1,1,-1) \end{aligned}\right\}$$ primitive RLVs (Eqn 2.36 pg 38)

$$\vec{G} = 2\pi/a\ (-h+k+l,\ h-k+l,\ h+k-l)$$

There are 14 G's to consider

1-3) (100), (010), (001) : $|\vec{G}| = \frac{2\pi}{a}\sqrt{3}$

4-6) (-100) (0-10) (00-1) " " "

7-8) (111), (-1-1-1) $|\vec{G}| = \frac{2\pi}{a}\sqrt{3}$

9-11) (011), (101), (110) $\frac{4\pi}{a}$

12-14) (0-1-1), (-10-1), (-1-10) $\frac{4\pi}{a}$

Notation: G_{hkl}

$$\text{ie } G_{100} = \frac{2\pi}{a}(-1+0+0,\ 1-0+0,\ 1+0-0) = \frac{2\pi}{a}(-1,1,1)$$

$$G_{-100} = \frac{2\pi}{a}(1,-1,1)$$

etc.

Central eqn $$\Big(\underbrace{\frac{\hbar^2 k^2}{2m}}_{\text{"}\lambda_k\text{"}} - E\Big)C_k + \sum_G U_G C_{k-G} = 0$$

Only include the above G's ...

$$(\lambda_k - E)C_k + U_{100}\,C_{k-\frac{2\pi}{a}(-1,1,1)} + U_{-100}\,C_{k-\frac{2\pi}{a}(1,-1,-1)} + \cdots\ (12 \text{ more terms}) = 0$$

How to use Central Eqn, pg 2

This is a set of eqns, one for each k

$$\text{For } k=(0,0,0):\ (\lambda_{000}-E)C_{000}+U_{100}\underbrace{C_{(0,0,0)-\frac{2\pi}{a}(-1,1,1)}}_{\text{call it } C_{1-1-1}}+U_{-100}\underbrace{C_{(0,0,0)-\frac{2\pi}{a}(1,-1,-1)}}_{C_{-111}}+\dots(12\text{ terms})=0$$

$$\text{For } k=\frac{2\pi}{a}(1,0,0):\ (\lambda_{100}-E)C_{100}+U_{100}\underbrace{C_{\frac{2\pi}{a}[(1,0,0)-(-1,1,1)]}}_{C_{2-1-1}}+U_{-100}\underbrace{C_{\frac{2\pi}{a}[(1,0,0)-(1,-1,-1)}}_{C_{011}}+\dots(12\text{ terms})=0$$

C_{2-1-1} → Throw out! Assume unimportant

C_{011} → keep!

$$\sim C_{000}+(\lambda_{100}-E)C_{100}+\sim C_{010}+\sim C_{011}+\dots=0$$

$\lambda_{000}=0$

$\lambda_{100}=\frac{\hbar^2(\frac{2\pi}{a})^2}{2m}$

etc

$$\begin{pmatrix} \lambda_{000}-E & & \text{A bunch of} & \\ - & \lambda_{100}-E & U_{xyz}\text{ values} & \\ \text{A bunch of} & \lambda_{010}-E & & \\ U_{xyz}\text{ values} & & \lambda_{011}-E\ \dots & \\ & & & \lambda_{-1-10}-E \end{pmatrix}\begin{pmatrix} C_{000}\\ C_{100}\\ C_{010}\\ C_{011}\\ \vdots\\ C_{-1-10}\end{pmatrix}=0$$

$\det(\ \uparrow\ )=0$ → 14 different E values in terms of U_{xyz} values

Know/Model U → FT → solve matrix

For HW: Square Lattice 2D, given U

Kittel 7-6 → find 4 Fourier components

→ 2 equations w/ 5 terms each

↳ throw out 4

→ 2 x 2 matrix

★ Important Concept: Certain states get "mixed" together by the crystal potential day 30 pg 9

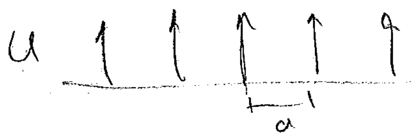
Solving Kronig-Penney w/ Central Eqn

Central Eqn $\left(\frac{\hbar^2 k^2}{2m} - E\right)C_k + \sum_G U_G C_{k-G} = 0$ used to solve for E as function of k

$\left(\frac{\hbar^2 k^2}{2m} - E\right)C_k$ ↓ Fourier coeff of the wavefunction

$\sum_G U_G C_{k-G}$ ↓ Fourier component of potential

Kronig Penney (delta function)



$$U(x) = Aa \sum_s \delta(x - sa)$$

Aa ↓ could just have be a constant, but Kittel doesn't. See why in a minute

Need to find U_G

$$U_G = \frac{1}{a}\int_{-a/2}^{a/2} \Big(\underbrace{Aa \sum_s \delta(x - sa)}_{\text{only one is in range: } \delta(x-0)}\Big) e^{+ikx}\, dx$$

e^{+ikx} ← or maybe $-ikx$, doesn't really matter in this case

$$= \frac{1}{a} Aa \quad e^{ik(0)}$$

$\underline{\underline{U_G = A}}$ All U_G's are equal for this case!

Skipped in class

Central Eqn:

$$\left(\frac{\hbar^2 k^2}{2m} - E\right)C_k + A \sum_G C_{k-G} = 0$$

$\hookrightarrow G = \frac{2\pi}{a}\cdot n$

$$\left(\frac{\hbar^2 k^2}{2m} - E\right)C_k + A \underbrace{\sum_n C_{k - \frac{2\pi n}{a}}}_{f(k - \frac{2\pi n}{a})} = 0$$

$$\left(\frac{\hbar^2 k^2}{2m} - E\right)C_k = -A\ f(k - \tfrac{2\pi n}{a})$$

Cool trick ... do $k' = k - \frac{2\pi n}{a}$, $k = k' + \frac{2\pi n}{a}$

Kronig-Penney via Central Eqn, pg 2

$$\left(\frac{\hbar^2}{2m}\left(k'+\frac{2\pi n}{a}\right)^2 - E\right) C_{k'+\frac{2\pi n}{a}} = -A\, f(k')$$

Now, rename $k' \to k$ again, solve for C

$$C_{k+\frac{2\pi n}{a}} = \frac{-A\, f(k)}{\frac{\hbar^2}{2m}\left(k+\frac{2\pi n}{a}\right)^2 - E}$$

Next cool trick: Sum both sides over all n

$$\underbrace{\sum_n C_{k+\frac{2\pi n}{a}}}_{} = -A\, f(k) \sum_n \frac{1}{\frac{\hbar^2}{2m}\left(k+\frac{2\pi n}{a}\right)^2 - E}$$

$= f\left(k+\frac{2\pi n}{a}\right)$

= same as $f(k)$

since n covers all values.

Divide by $f(k)$

$$1 = -A \sum_n \frac{1}{\frac{\hbar^2}{2m}\left(k+\frac{2\pi n}{a}\right)^2 - E}$$

$$\frac{\hbar^2}{2mA} = -\underbrace{\sum_n \frac{1}{\left(k+\frac{2\pi n}{a}\right)^2 - \frac{2mE}{\hbar^2}}}_{}$$

Kittel: minus sign there. I assume it doesn't matter.

→ difference of 2 squares
  → factor

→ partial fraction I think

→ $\sum_n \frac{1}{n\pi + x} = \frac{1}{\tan x}$

→ "trig manipulation"

"And then a miracle occurs"

$$\frac{\hbar^2}{2mA} = \frac{-a^2 \sin\sqrt{\frac{2mE}{\hbar^2}}\, a}{2\sqrt{\frac{2mE}{\hbar^2}}\, a \left(\cos ka - \cos\sqrt{\frac{2mE}{\hbar^2}}\, a\right)}$$

Let $K = \sqrt{\frac{2mE}{\hbar^2}}$, multiply over

$$\boxed{\overset{}{\underset{\substack{\uparrow \\ \text{little } k}}{\cos ka}} = \frac{mAa^2}{2\hbar^2}\,\frac{1}{Ka}\,\sin Ka + \cos KA}$$

gives you same relationship between k and E as done previously!

Skipped this