

Example: How the central eqn might be used. (from Peter's final exam)

- GaAs crystal, assumed only waves which couple to a given state are those with V_G components for $|G| = \frac{2\pi}{a}$. 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

$$\vec{b}_1 = \frac{2\pi}{a} (-1, 1, 1)$$

$$\vec{b}_2 = \frac{2\pi}{a} (1, -1, 1)$$

$$\vec{b}_3 = \frac{2\pi}{a} (1, 1, -1)$$

primitive
RLVs

(Eqn 2.36 pg 38)

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

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}

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

↓
"λ_k"

Only include the above G 's ...

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

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How to use Central Eqn, pg 2

This is a set of eqns, one for each k

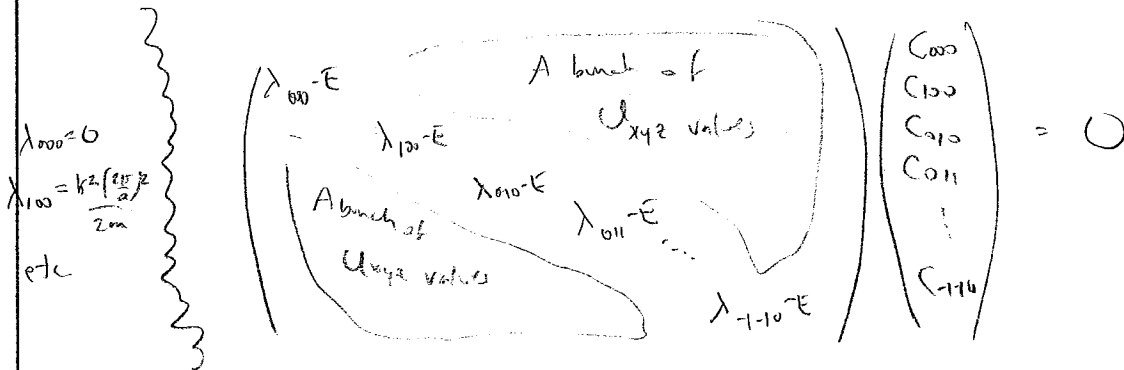
$$\text{For } k=(0,0,p): (\lambda_{000}-E)C_{000} + \underbrace{U_{100} C_{(0,0,0)-\frac{2\pi}{a}(-1,1,1)}}_{\text{call it } C_{-1-1}} + \underbrace{U_{-100} C_{(0,0,0)-\frac{2\pi}{a}(1,-1,1)}}_{C_{-111}} + \dots (12 \text{ terms}) = 0$$

$$\text{For } k=\frac{2\pi}{a}(1,0,p): (\lambda_{100}-E)C_{100} + \underbrace{U_{100} C_{\frac{2\pi}{a}[(1,0,0)-(1,1,1)]}}_{C_{2-11}} + \underbrace{U_{-100} C_{\frac{2\pi}{a}[(1,0,0)-(1,-1,1)]}}_{C_{011}} + \dots (12 \text{ terms}) = 0$$

↓
Throw out!
Assume unimportant

↓
keep!

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



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

Known/Model $U \rightarrow$ FT \rightarrow solve matrix

For HW: Square Lattice 2D, given U

Kittel 7-6

\rightarrow find 4 Fourier components

\rightarrow 2 equations w/ 5 terms each

\hookrightarrow throw ~~out~~ out 4

\rightarrow 2x2 matrix

Important concept: certain states get "mixed" together

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Solving Kronig-Penney w/ Central Eqn

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

\downarrow Fourier coeff of the wavefunction \downarrow Fourier component of potential

used to solve for E as function of k

Kronig Penney (Delta function)



$U(x) = A a \sum_s \delta(x - sa)$

\downarrow could just write in a constant, but k still doesn't see why in a minute

Need to find U_G

$$U_G = \frac{1}{a} \int_{-a/2}^{a/2} \left(A a \sum_s \delta(x - sa) \right) e^{+ikx} dx$$

$\underbrace{\hspace{10em}}$ output is in range of $\delta(x-0)$

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

or maybe $-ikx$, doesn't really matter in this case

$U_G = A$ All U_G 's are equal for this case!

Central Eqn:

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

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

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

$\underbrace{\hspace{10em}}$ $f(k - \frac{2\pi n}{a})$

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

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

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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 $k' \rightarrow k$ 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

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

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

= same as f(k)

since n covers all values.

Divide by f(k)

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

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

little minus sign there. I assume it doesn't matter.

→ difference of 2 squares (to factor)

→ partial fractions I think

$$\rightarrow \sum_n \frac{1}{n^2 + x} = \frac{1}{\tan x}$$

→ "trig manipulation"

"And then a miracle occurs"

$$\frac{\hbar^2}{2m A} = -a^2 \sin \sqrt{\frac{2mE}{\hbar^2}} a \cdot \frac{1}{2\sqrt{\frac{2mE}{\hbar^2}} a (\cos ka - \cos \sqrt{\frac{2mE}{\hbar^2}} a)}$$

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

$$\cos ka = \frac{m A a^2}{2 \hbar^2 K a} \sin Ka + \cos Ka$$

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

Skipped this