8/29 pg 1

Band Structure

{ handout w/ Si + GaAs bands }

Why are curves so complicated

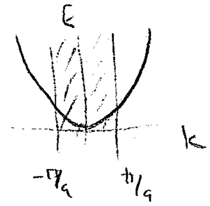
(1) Periodicity of lattice, structures + symmetries → Geometrical Effect

(2) Details of $U(x)$ aka $U(\vec{r})$ → QM effect
Effect of "crystal potential" (like Kronig Penney bandgaps)

Tackle #1 first (kittel tackles #2 first)

Empty Lattice Model

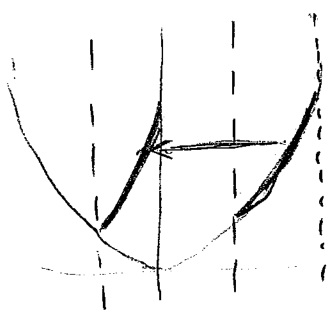
1D: $E = \frac{\hbar^2 k^2}{2m}$



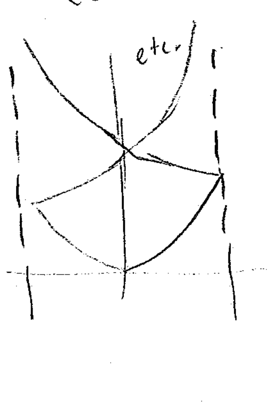
Two ways of plotting: 1) "extended zone scheme", plot as parabola
2) "reduced zone scheme", plot (like phonons) 1st BZ only, bringing back by RLVs as needed.

~~Let's do this, presenting that the motivation isn't guiding things as it was for phonons~~

already did this for 1D



etc.



1D fairly easy to envision

3D: harder! Do simple cubic case only.

Book/class: 100 direction only

HW: 111 direction

Empty lattice, cont.

$$E = \frac{\hbar^2 k^2}{2m} \longrightarrow = \frac{\hbar^2 (\vec{k}+\vec{G})^2}{2m}$$

$$= \frac{\hbar^2}{2m}\left[(k_x+G_x)^2 + (k_y+G_y)^2 + (k_z+G_z)^2 \right]$$

Looking for things that end up in 100 direction

Go over
Handout for 100, simple cubic
w/ Mathematica

Central Eqn (derivation) $-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + U(x)\psi = E\psi$

periodic ... expand in Fourier series

(like when we did FT of lattice itself back in chapter 2)

$$U(\vec{r}) = \sum_{\vec{G}} U_{\vec{G}}\, e^{i\vec{G}\cdot\vec{r}}$$

Fourier components, also given symbol U ... but don't get confused!

or 1D: $U(x) = \sum_G U_G e^{iGx}$

plug into Schrodinger

Also write ψ as linear comb of free electron solutions

$$\psi(x) = \sum_k C_k e^{ikx}$$

plug into Schrodinger

$\frac{d}{dx} \to ik$

periodic bndy cond. $\psi(0) = 0$ and $\psi(L) = 0$

physical size (length) of crystal

$\Rightarrow k = \frac{2\pi n}{L}$

Then ...

$$-\frac{\hbar^2}{2m}(-k^2)\sum_k C_k e^{ikx} + \sum_G \sum_k U_G C_k e^{i(k+G)x} = E\sum_k C_k e^{ikx}$$

$k' = k+G$

$$\sum_G \sum_{k'} U_G C_{k'-G} e^{ik'x}$$

rename $k' \to k$

Equate each coeff of e^{ikx}:

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

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

Careful! infinite # of G's
- infinite (nearly) # of k's
- infinite ~~amt~~ # of unknown C's

$\hbar k$ = "crystal momentum of electron"

Again, a lot like an infinite eigenvalue matrix eqn!
takes place of Schrodinger diff eqn.

How to use: 1) Calculate Fourier coeffs of U
2) Truncate to some appropriate number ("two to four" will suffice) ← Write down
3) Solve matrix eqn to determine C's
4) Then you have ψ (and easily E?)