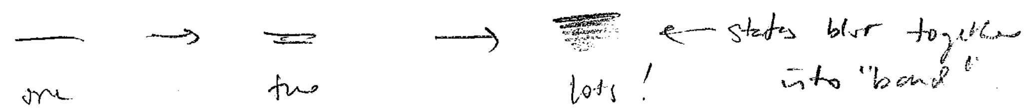
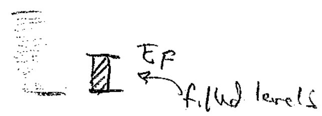
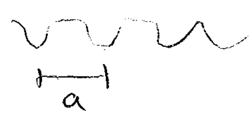




Bloch Theorem

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

If V is periodic: $V(x+na) = V(x)$



then: (perhaps) $\psi(x+na) = \psi(x)$?

No → too strong a condition

$$\psi(x+na) = e^{i\alpha}\psi(x)$$

off by a phase factor is OK, since $|\psi|^2$ is what's real

Actual Thm: $\boxed{\psi(x) = e^{ikx}u_k(x) \quad \text{with } u_k(x) = u_k(x+na)}$

Demonstrate: $\psi(x+na) = \underbrace{e^{ik(x+na)}}_{e^{ikx}e^{ikna}}\underbrace{u_k(x+na)}_{=u_k(x)}$

$= \psi(x)\cdot e^{ikna}$ ✓ it worked!

important: this is the phase factor.

(that's half the proof, anyway. still need to prove other direction: only this form works)

(From slides pg 82-83)

Given Bloch theorem $\psi = u_k(x) e^{i(kx)}$

periodic $u_k(x) = u(x + sa)$

different for each value of k

→ Every wavefunction is associated
- with some free electron wavefunction e^{ikx}

Can label every wavefunction with k, even for electrons which are not free

Consider wavefunction labeled w/ k' = outside 1st BZ

write $k' = k - G$

k: inside 1st BZ

G: some RLV $= \left(\frac{2\pi}{a}\right) \times n$ (some n)

$$\psi = u_{k'}(x) e^{i(k-G)x}$$

$$u_{k'}(x) e^{ikx} e^{-iGx}$$

$e^{-iGx} \rightarrow e^{i\left(-\frac{2\pi n x}{a}\right)}$ → periodic in x, period a

lump together

$$= \underbrace{u_{n,k}(x) e^{ikx}}$$

Bloch function with k inside first BZ

w/ Different u function → hence label "n", to distinguish it from $u_k(x)$

Since all electrons can be labeled with wave vectors k inside 1st BZ, we can restrict x-axis to 1st BZ in all plots.
(n becomes index of bands)

(From Stokes pg 73-74)

Also like phonons, states separated by $\frac{2\pi}{L}$ ← length of physical crystal

Proof 1: Force $\psi = 0$ on bndys

Then it's "particle in infinite square well"
(very wide well)

$$A \sin \frac{n\pi x}{L} \rightarrow k = \frac{n\pi}{L}$$

Spacing is $\frac{\pi}{L}$

But ... this includes positive values of k only
To include negative k's w/o changing total N,
must "stretch" out by factor of 2

Proof 2 Force periodic bndy conditions (because surface = unimportant)

$$\psi(x+L) = \psi(x)$$

$$\psi(x) = Ae^{i2n\pi x/L} \rightarrow k = \frac{2n\pi}{L}$$

Spacing is $\frac{2\pi}{L}$ ✓

includes both + and − values of k ✓
and direction of k can be
used to indicate electron velocity