Lecture 5 - Band structure

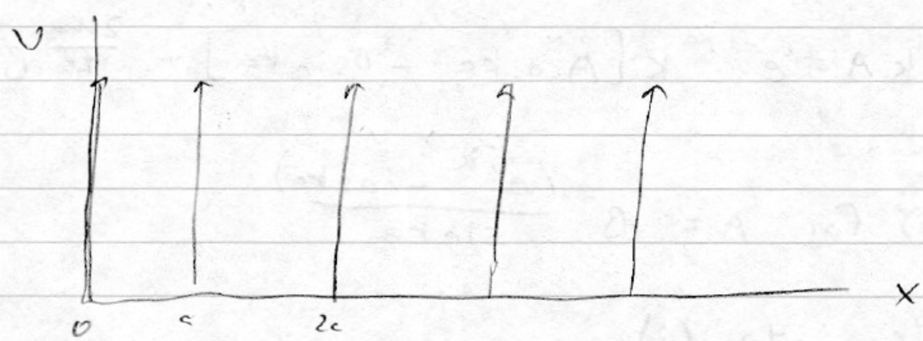
Last time started to look at more realistic model
for electrons in a crystal
→ include interactions with ion cores

Introduced Bloch's Theorem:
If potential $U(x+a) = U(x)$

Then single-particle energy eigenstates $\psi_k(x+a) = e^{ika}\psi(x)$

So in a crystal, only need to solve Sch Eqn
for $0 \le x < a$, get rest by translation.

Example: $U(x) = \alpha \sum_j \delta(x - ja)$



Not a model for a real crystal, just the
simplest periodic potential we can find.

Solve for states:

For $0 < x < a$, particle is free

$\psi(x) = A\sin kx + B\cos kx \qquad E = \frac{\hbar^2 k^2}{2m}$

Need correct continuity at $x=0$

For $-a<x<0$, have
$$\psi(x) = e^{-iKa}\left[A\sin k(x+a) + B\cos k(x+a)\right]$$

where K is unknown function of k to be determined

Need $\psi(0+) = \psi(0-)$

So

(1) $$B = e^{-iKa}(A\sin ka + B\cos ka)$$

and also $$\left.\frac{d\psi}{dx}\right|_{0+} = \left.\frac{d\psi}{dx}\right|_{0-} + \frac{2m\alpha}{\hbar^2}\psi(0)$$

discontinuity from δ-function potential

So

(2) $$kA = e^{-iKa}k\left[A\cos ka - B\sin ka\right] + \frac{2m\alpha}{\hbar^2}B$$

Solve (1) for $A = B\dfrac{(e^{iKa} - \cos ka)}{\sin ka}$

Substitute into (2)

(Also cancel overall B and clear $\sin ka$):

$$k(e^{iKa} - \cos ka) = e^{-iKa}k\left[(e^{iKa} - \cos ka)\cos ka - \sin^2 ka\right] + \frac{2m\alpha}{\hbar^2}\sin ka$$

$$= e^{-iKa}k\left[e^{iKa}\cos ka - 1\right] + \frac{2m\alpha}{\hbar^2}\sin ka$$

$$e^{iKa} - \cos ka = \cos ka - e^{-iKa} + \frac{2m\alpha}{\hbar^2 k}\sin ka$$

$$\boxed{\cos Ka = \cos ka + \frac{m\alpha}{\hbar^2 k}\sin ka}$$

Implicitly gives $k(K) \Rightarrow E(K)$
(recall K is our quantum number, can take any value)

Too bad we can't solve it explicitly!

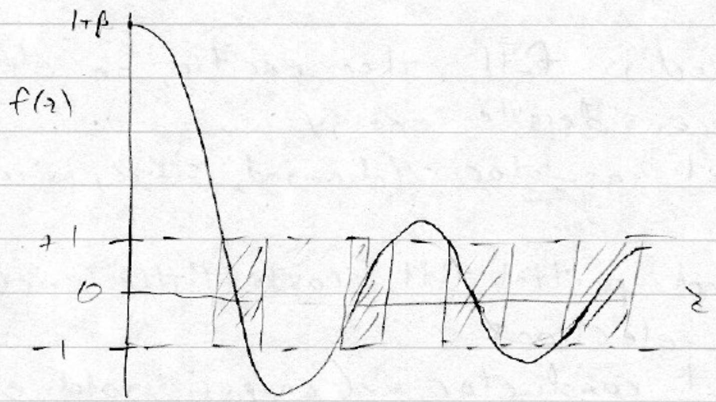
Rewrite $\cos Ka = f(z)$

$$f(z) = \cos z + \beta \frac{\sin z}{z}$$

$$z = ka \qquad \beta = \frac{m\alpha a}{\hbar^2}$$

→ strength of potential

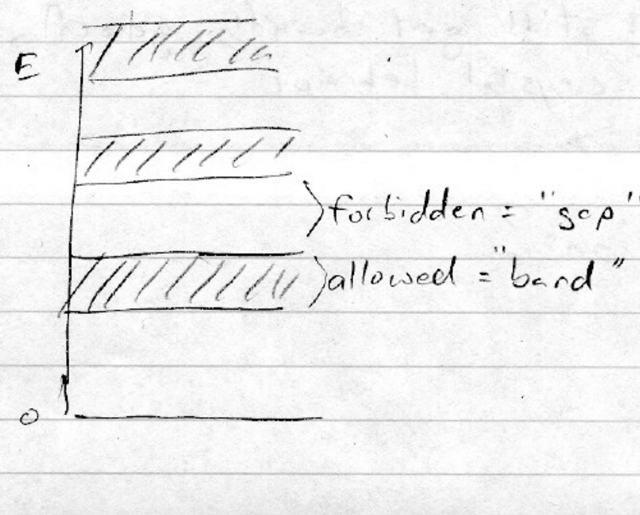
Plot



(web supplement)

No solution unless $|f(z)| < 1$
→ only certain values of z allowed
→ only certain values of k
→ certain values of E

Draw like:



This gives energies of our single particle states

See Griffiths for details

For finite system length ℓ_x, each band breaks up into discrete states $\Delta K \sim \frac{\pi}{\ell_x}$

Turns out to be N states per band, N = # of atoms
(Really 2N states per band, including spin)

So if each atom donates q electrons,
for q = even, fill up q/2 bands
for q = odd, top band is half full.
"valence band"

If valence band is full, then exciting an electron costs considerable energy
→ electrical insulator (diamond, silica, mica, etc)

If valence band partial fill, costs little energy to excite electrons
→ electrical conductor (copper, gold, etc)

For more realistic potentials, relation between K and k is more complicated

But still get bands, good description of crystal behavior

→ Questions?