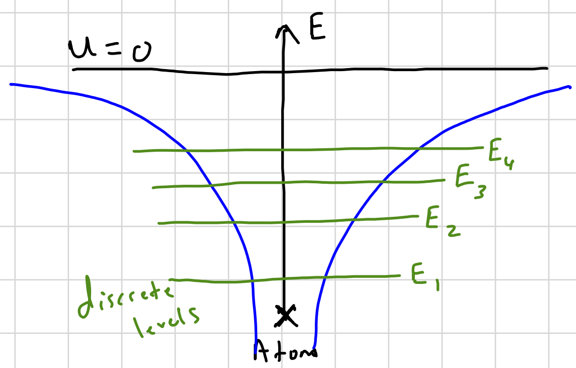
Lecture # 4 — Quantum Theory of Solids (cont.)

Kronig-Penney model

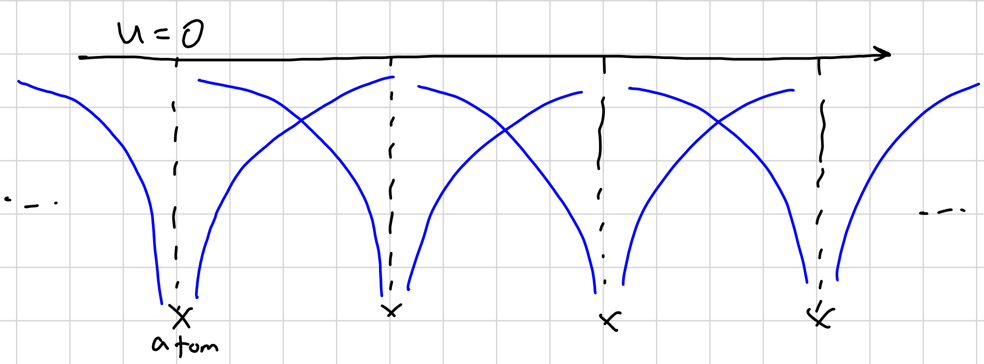
Energy bands tell us where e^-'s are allowed to be, but what dictates how they move from one place to another?

→ most influential is their attraction to the atomic nuclei

Individual Atom:

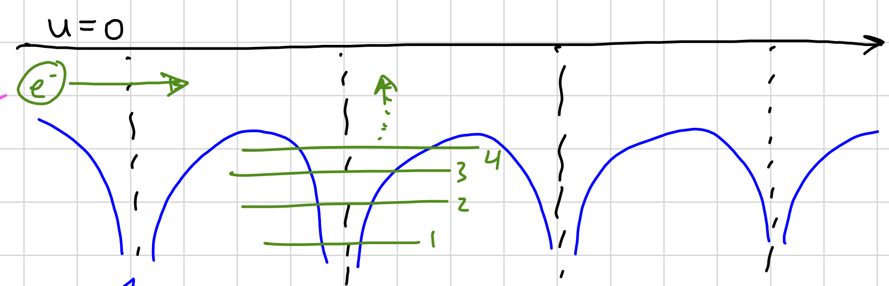


1D Lattice



e^- moving through the lattice, experiencing a "periodic potential"

Net potential profile



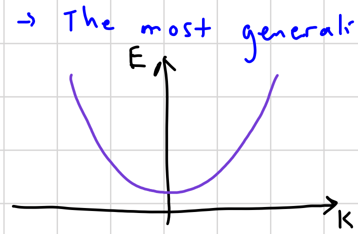
• Kronig Penney model approximates with square step functions and solves Schrödinger's eqn.

What is the result?

→ A solution for energy of an e^- with relation to k → "wave number" and the momentum (p) of the e^- is: $\boxed{p = \hbar k}$, $E = \frac{p^2}{2m}$

→ This solution/relation between E and K is also known as a "dispersion relation"

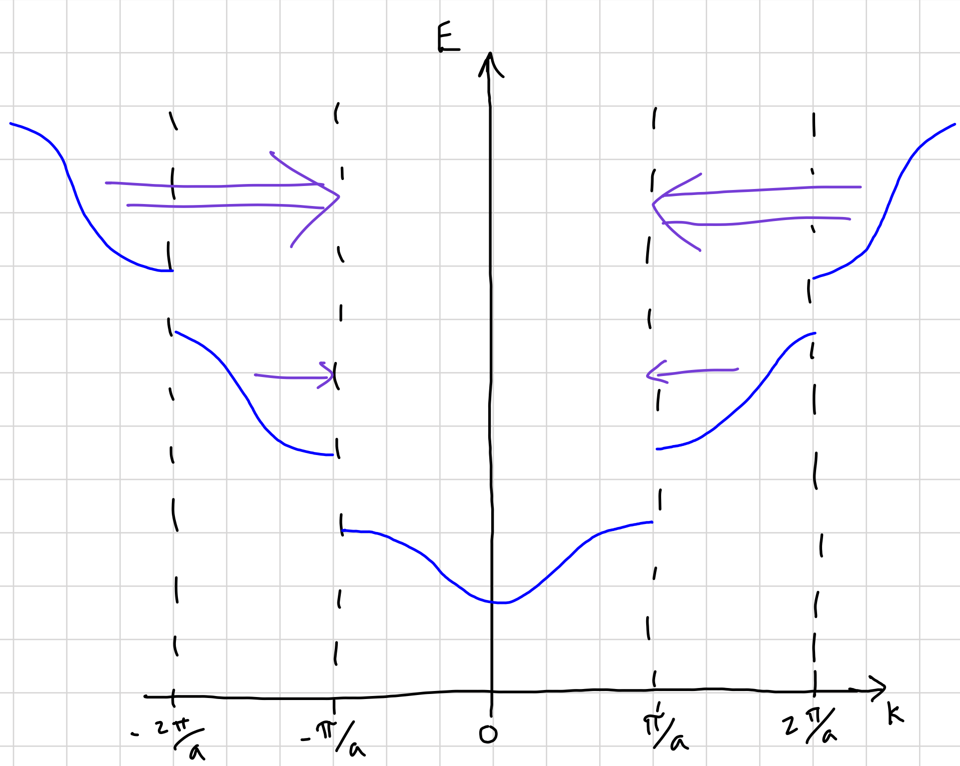
→ The most generalized solution gives this relation:



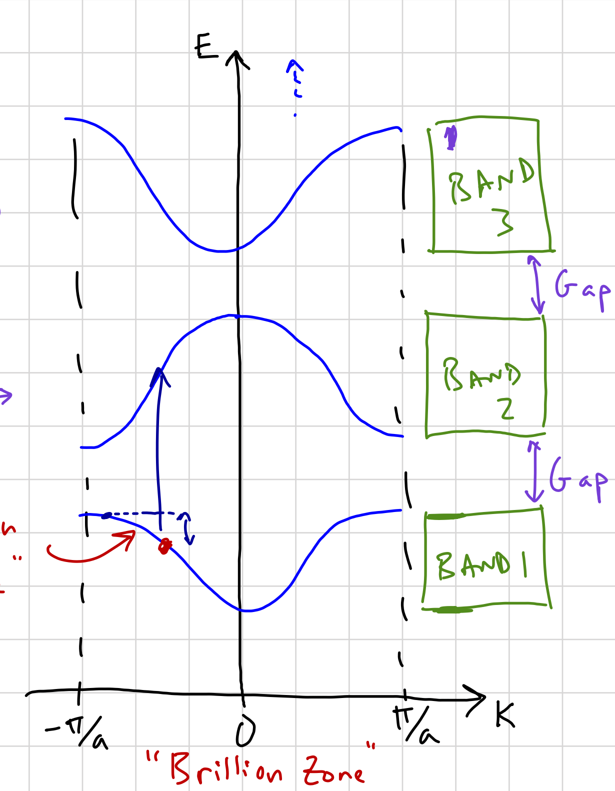
$$\boxed{E = \frac{\hbar^2 k^2}{2m}}$$

parabolic dispersion relation for "free particle" (NOT in a 1D periodic lattice!)

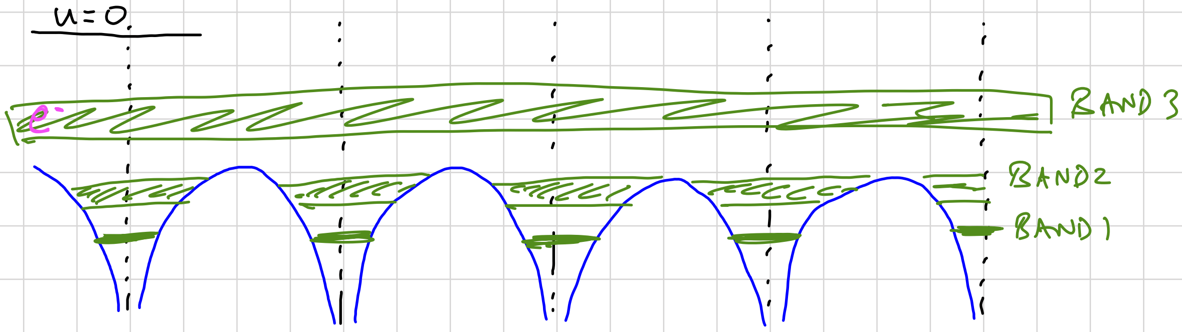
If the periodic conditions of the crystal are applied, then the "allowed" values of K for which the wave eqn. has a solution give you your E-K diagram:



Due to periodicity of 2π, can translate these allowed energy bands to a reduced K-space representation →

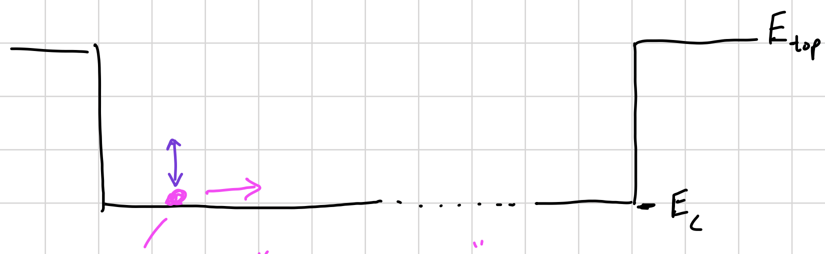


Visualizing these energy bands in a crystal:



Generally, an e^- will be in an "upper" or higher energy band and thus is effectively like a particle-in-a-box with:

$$\boxed{E = \frac{\hbar^2 k^2}{2m}, \quad k = \sqrt{\frac{2mE}{\hbar^2}}}$$



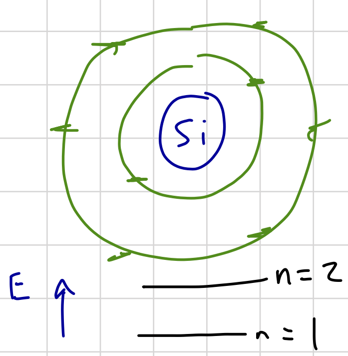
effectively a "free particle" in a well with periodic B.C.'s

Comes from time-indepent S.E.:

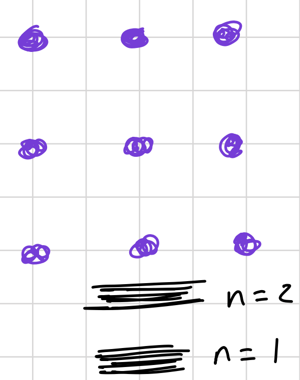
$$\frac{\partial^2 \psi}{\partial x^2} + \underbrace{\frac{2mE}{\hbar^2}}_{k^2}\psi = 0$$

→ Where are e^-'s allowed to be in a semiconductor crystal?

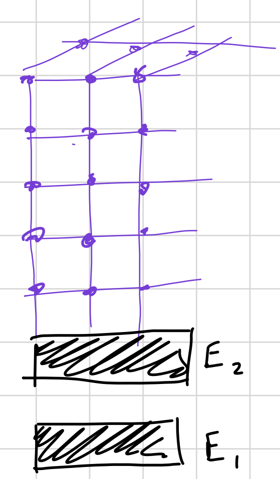
RECAP:



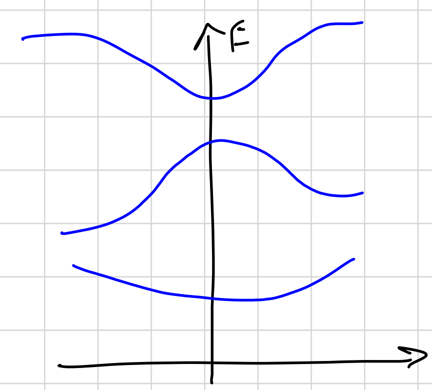
Atom: e^-'s in orbitals



N atoms brought together causes E-levels to split N times



Energy bands are formed in atomic crystals



Solving wave eqn. in periodic crystal yields relationship between E-k

wave number (crystallographic direction vector)

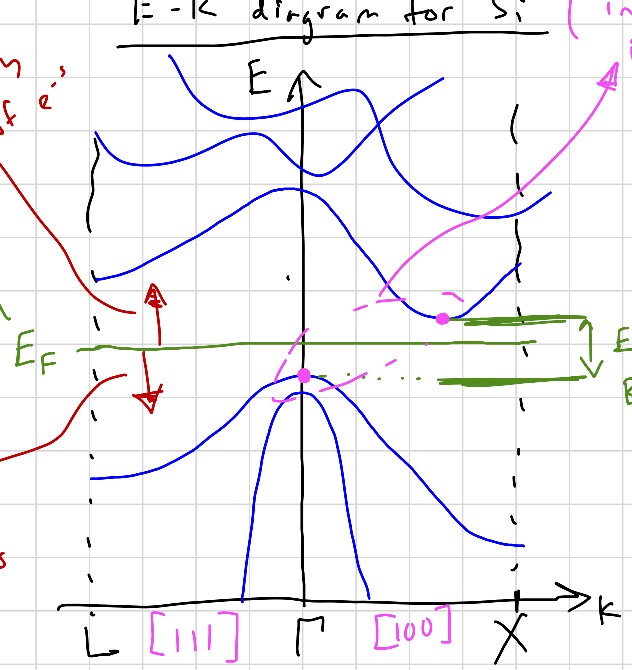
- Thus far this was developed for 1D, how does it look in 3-D crystal?

E-k diagram for Si ("indirect" Band gap)

all states are empty of e^-'s

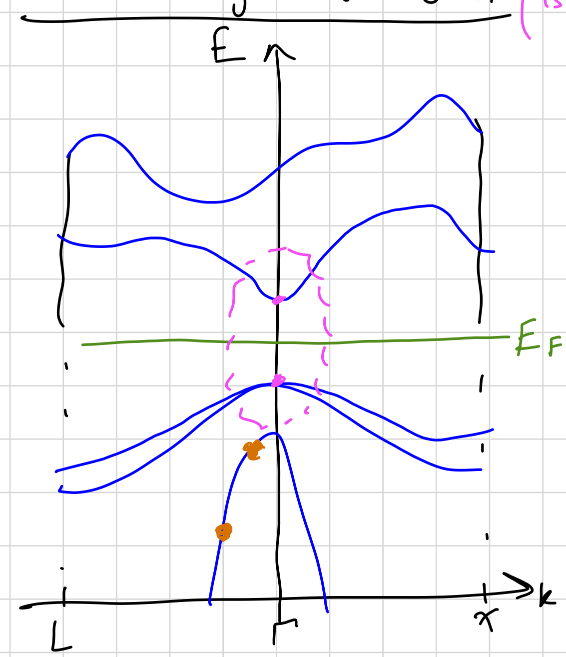
"Fermi" level

all states are filled with e^-'s



Energy Band gap

E-k diagram for GaAs (direct Band gap)



-> What properties does an e^- have?

-> Effective mass (m^*) Consider parabolic E-k relation: $E = \frac{\hbar^2 k^2}{2m}$

$$\frac{dE}{dk} = \frac{\hbar^2 k}{m} = \frac{\hbar p}{m}$$

relate p to velocity by $v = \frac{p}{m}$: $\boxed{\frac{1}{\hbar}\frac{dE}{dk} = \frac{p}{m} = v}$

take 2^{nd} derivative: $\frac{d^2E}{dk^2} = \frac{\hbar^2}{m} \rightarrow \boxed{m^* = \hbar^2 \left(\frac{d^2E}{dk^2}\right)^{-1}}$

☆ For a free e^- mass is constant, but when bound in crystal with periodic potential it depends on inverse of E-k curvature

m^* ties classical world to quantum: $F = ma = -eE$ (see textbook)

charge

electric field