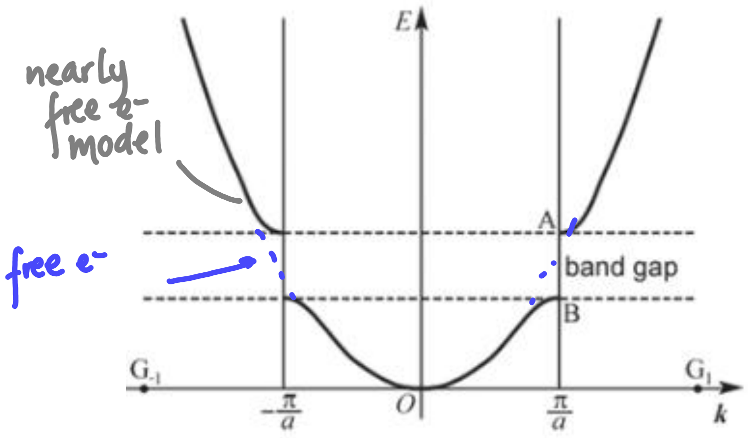
Electronic Band Structure

Lecture 4

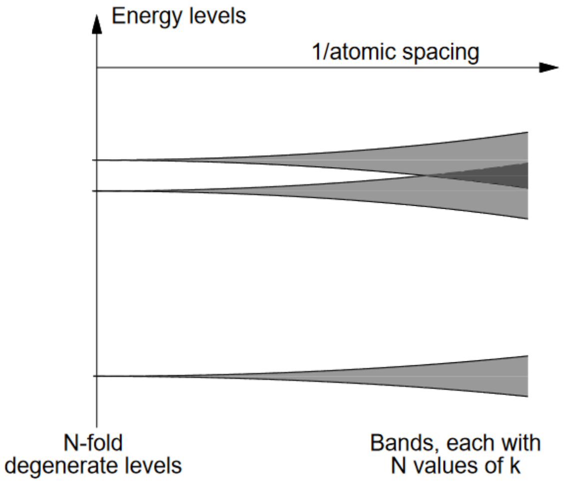
Nearly free electron *vs.* tight binding model



Nearly free e- model:

start: continue and parabolic band of free e-

Gap: attribute to Bragg reflexions at zone boundaries



Tight binding model

start: discrete levels of isolated atoms

Bands emerge due to progressive splitting caused by the interaction with other atoms in the crystal (e- keep the "character" of original bands)

1D: $E(K) = E_d - 2t\cos Ka$

Periodic Table of the Fermi Surfaces of Elemental Solids

http://www.phys.ufl.edu/fermisurface

Tat-Sang Choy, Jeffery Naset , Selman Hershfield, and Christopher Stanton
Physics Department, University of Florida

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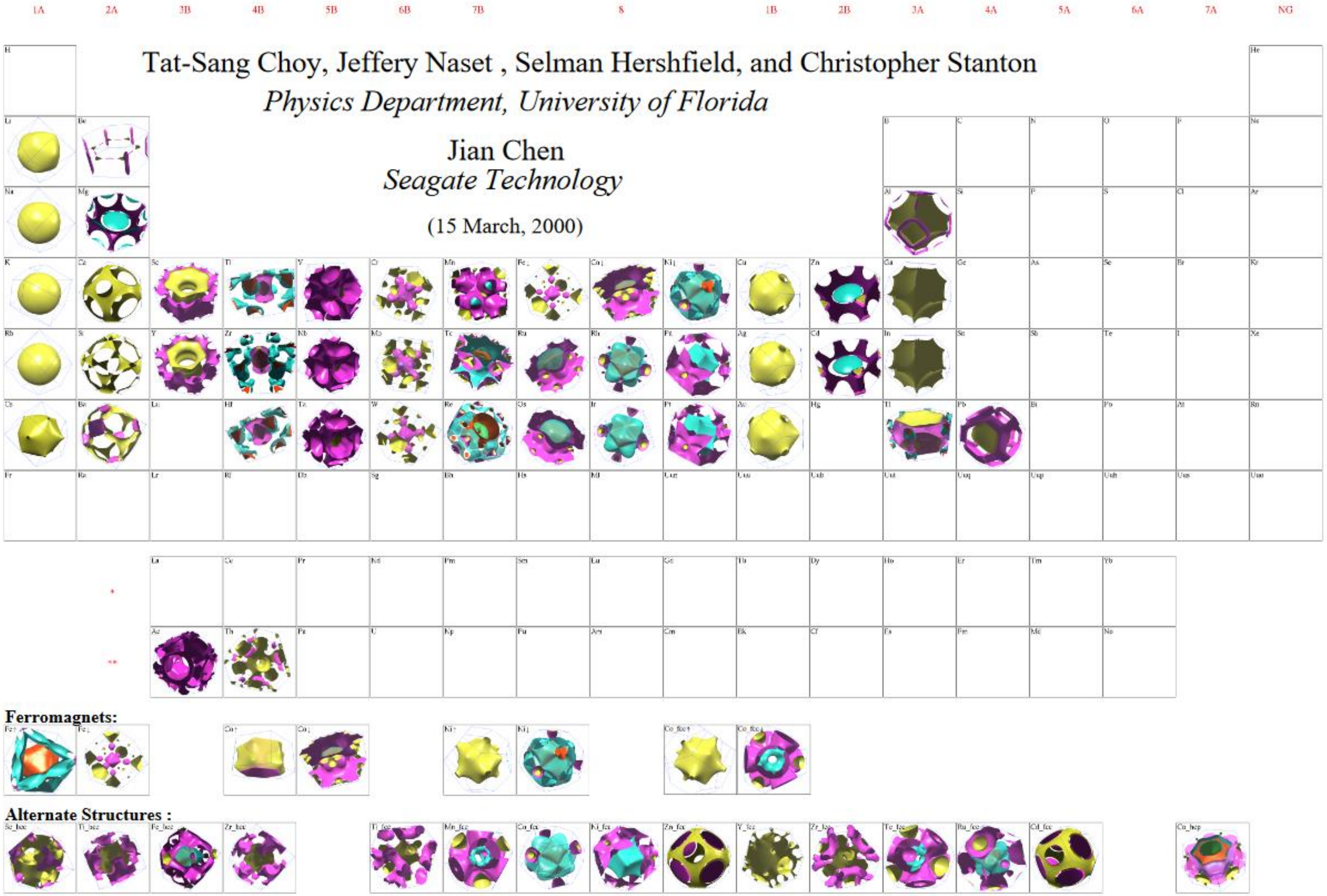
(15 March, 2000)



Source of tight binding parameters (except for fcc Co ferromagnet): D.A. Papaconstantopoulos, *Handbook of the band structure of elemental solids*, Plenum 1986.

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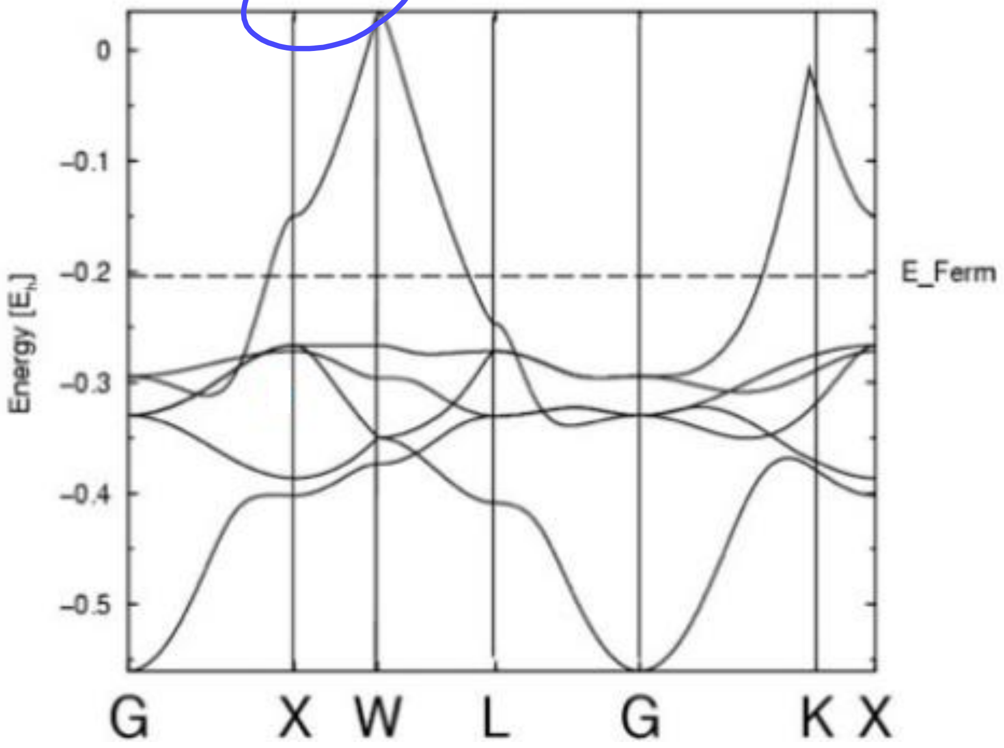
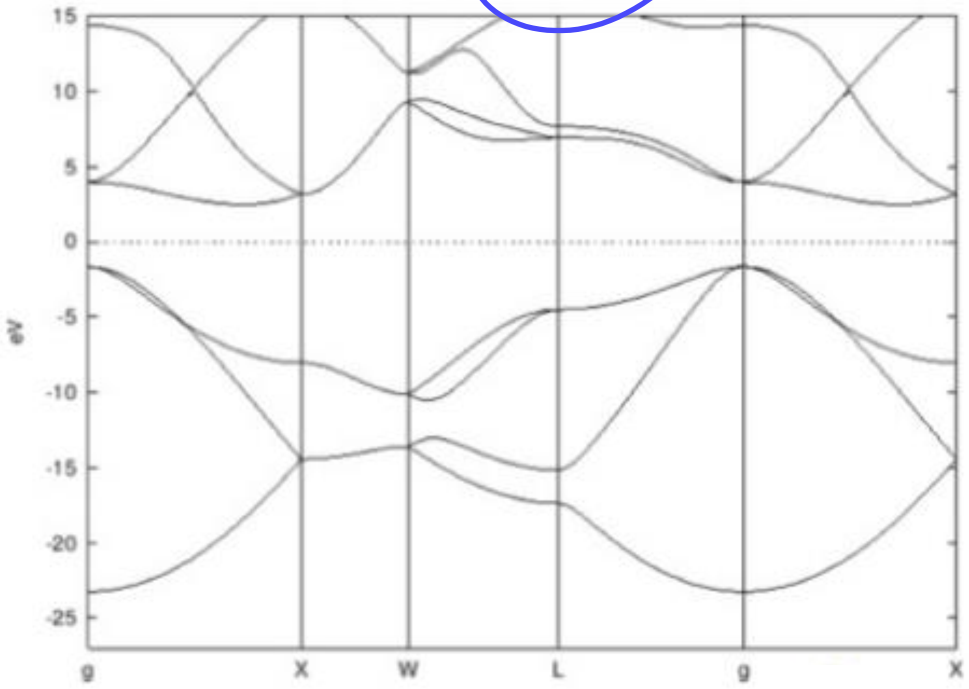
Quiz

Metal or insulator?



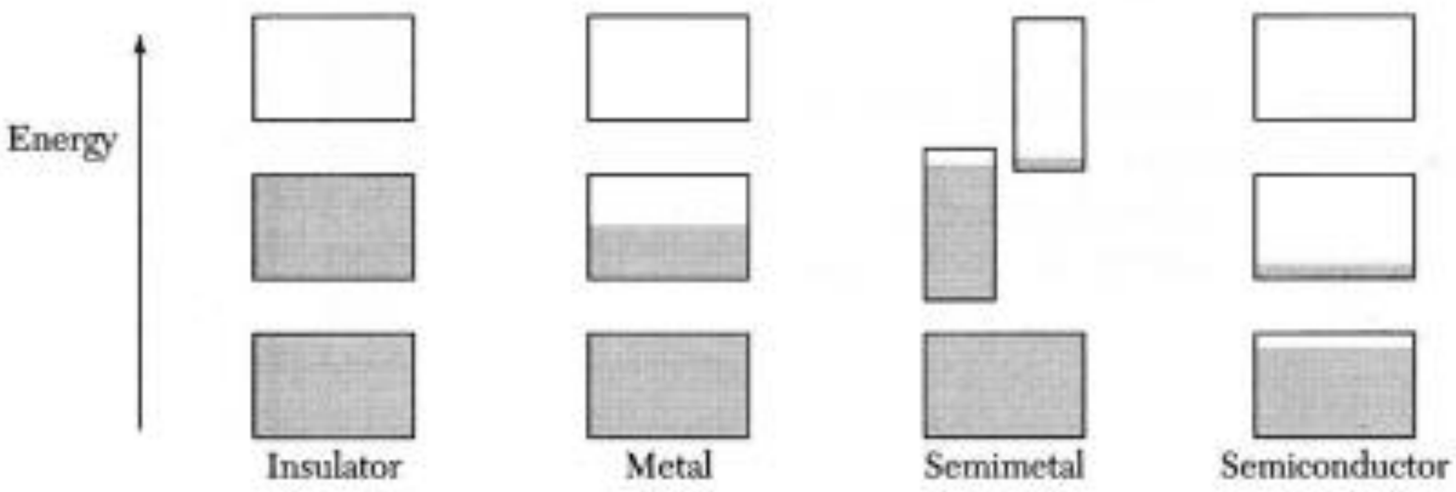
Metal or insulator?



Quiz

Does a semiconductor have a Fermi surface?

Does a semimetal have a Fermi surface?



Equations of motion and effective mass

$\hbar\vec{k}$ is not the momentum!

free e^-: plane waves $\phi_K = e^{i\bar{K}\bar{r}}$

$$\vec{p}\,\phi_K(\bar{r}) = -i\hbar\bar{\nabla} e^{iKr} = \hbar\bar{K} e^{i\bar{K}\bar{r}} = \underbrace{\hbar\vec{K}}_{\text{eigenvalue}}\,\phi_K(\bar{r})$$

Bloch theorem $\psi_K(\bar{r}) = e^{i\bar{K}\bar{r}} u_K(r)$

$$\vec{p}\,\psi_K(\bar{r}) = -i\hbar\nabla e^{iKr} u_K(r) = \underbrace{\hbar\bar{K}\,\psi_K(r)}\; - \underbrace{e^{iKr}\, i\hbar\nabla u_K(r)}$$

$\Rightarrow$ $\hbar\vec{K}$ is a crystal momentum

it is better to think $\bar{K}$ as a quantum number of 3 components which indices a Bloch state (= an electronic state within a band

$$\underbrace{\vec{K}}_{e} + \underbrace{\vec{K}}_{\text{phonon}} = \underbrace{\vec{K}'}_{e^- \text{ after collision}} + \underbrace{\vec{G}}_{\text{R.L. vector}}$$

when $G=0$: normal process

$G \neq 0$: Umklapp

Group velocity

Bloch state : e- wavefunction is defined as a superposition of plane waves

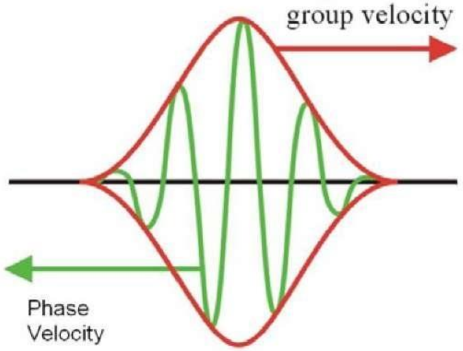
group velocity $v_g = \frac{d\omega}{dK} = \frac{1}{\hbar}\frac{dE}{dK}$

$\uparrow$ $E = \hbar\omega$

$$\vec{v} = \frac{1}{\hbar}\nabla_K E$$

group velocity: movement of e- in real space

the effects of the crystal on the motion are contained in the dispersion relation



Equations of movement

1D $\quad f$ = external force applied to a band e^- (wavepacket)

work done during time δt : $\delta E = f \cdot v \delta t$

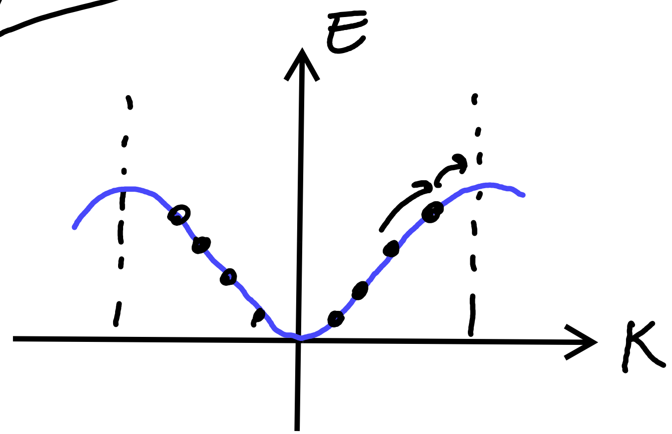
$$\delta E = \frac{\partial E}{\partial K} dK = \hbar v \delta K$$

$$v = \frac{1}{\hbar} \nabla_K E = \frac{1}{\hbar} \frac{dE}{dK}$$

$$f v \delta t = \hbar v \delta K$$

$$f = \hbar \frac{dK}{dt}$$

3D
$$\vec{f} = \hbar \frac{d\vec{K}}{dt}$$



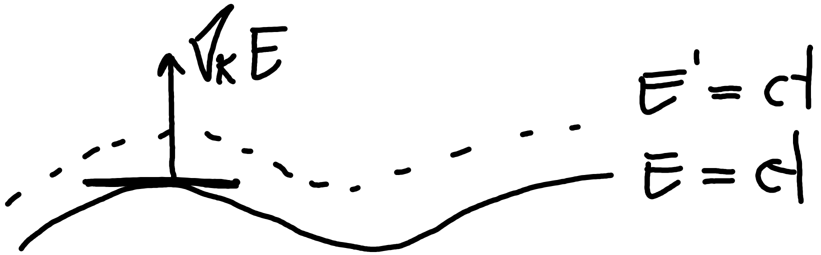
Ex Movement of $\vec{K}$ when a magnetic field is applied

$$\vec{f} = -e\bar{v}_g \times \bar{B} = \hbar \frac{d\bar{K}}{dt}$$

$$\bar{v}_g = \frac{1}{\hbar} \nabla_K E$$

$$\boxed{\frac{d\bar{K}}{dt} = -\frac{e}{\hbar^2}\left(\bar{\nabla}_K E \times \bar{B}\right)}$$

$d\bar{K}$ is $\perp \nabla_K E$ aua $\perp B$



* e^- moves on a surface of constant energy

Effective mass

let's calculate the acceleration of our "wavepacket"

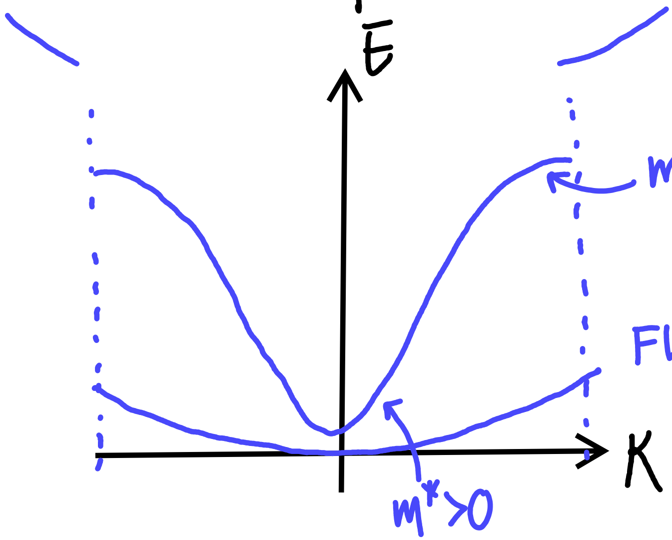
$$\frac{dv}{dt} = \frac{d}{dt}\left(\frac{1}{\hbar}\frac{dE}{dK}\right) = \frac{d}{dK}\frac{dK}{dt}\left(\frac{1}{\hbar}\frac{dE}{dK}\right) = \frac{1}{\hbar}\frac{d^2E}{dK^2}\cdot\underbrace{\frac{dK}{dt}}_{f/\hbar}$$

$$\Rightarrow \frac{dv}{dt} = \frac{1}{\hbar^2}\frac{d^2E}{dK^2}\cdot f$$

it looks quite similar to the classical formula $f = m^* a$

with $$\boxed{\frac{1}{m^*} = \frac{1}{\hbar^2}\frac{d^2E}{dK^2}}$$

m^* is the EFFECTIVE MASS

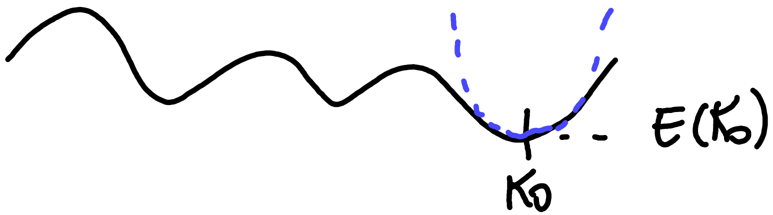


in 3D (anisotropic electron energy surfaces)

$$\underbrace{\frac{1}{(m^*)_{ij}}}_{\text{tensor}} = \frac{1}{\hbar^2}\frac{\partial^2(E(K))}{\partial K_i \partial K_j}$$

in general, m^* depends on energy, but:

Often we deal with almost filled or almost empty bands, close to a max or min of $E(K)$, series of Taylor:

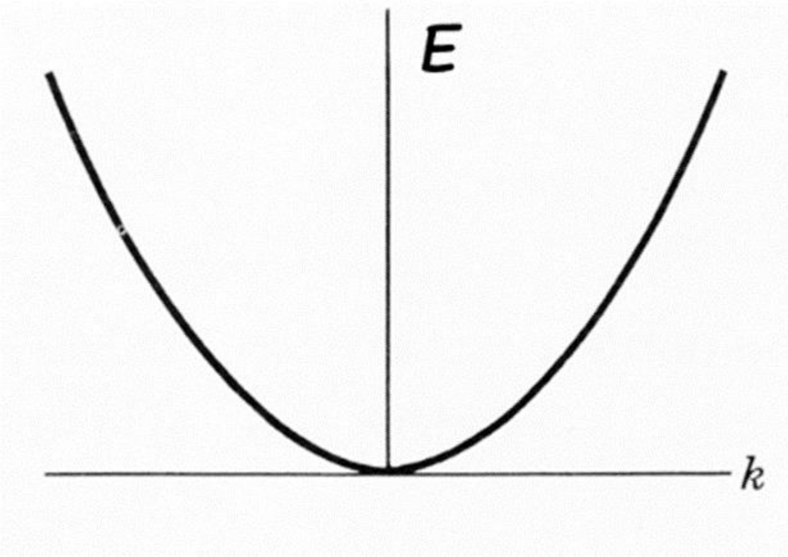


$$E(K) = E(K_0) + \underbrace{\frac{dE}{dK}\Big|_{K_0}}_{=0 \text{ @ max or min}} (K-K_0) + \frac{1}{2} \underbrace{\frac{d^2E}{dK^2}}_{=\hbar^2/m^*}\Big|_{K_0} (K-K_0)^2 + \dots$$

$$\Rightarrow E(K) = E(K_0) + \frac{\hbar^2}{2m^*}(K-K_0)^2 \qquad E(K) \approx \text{parabolic}$$

So, in these regions (close to max/min of bands) the energy can be approx. by that of a free particle of effective mass m^*

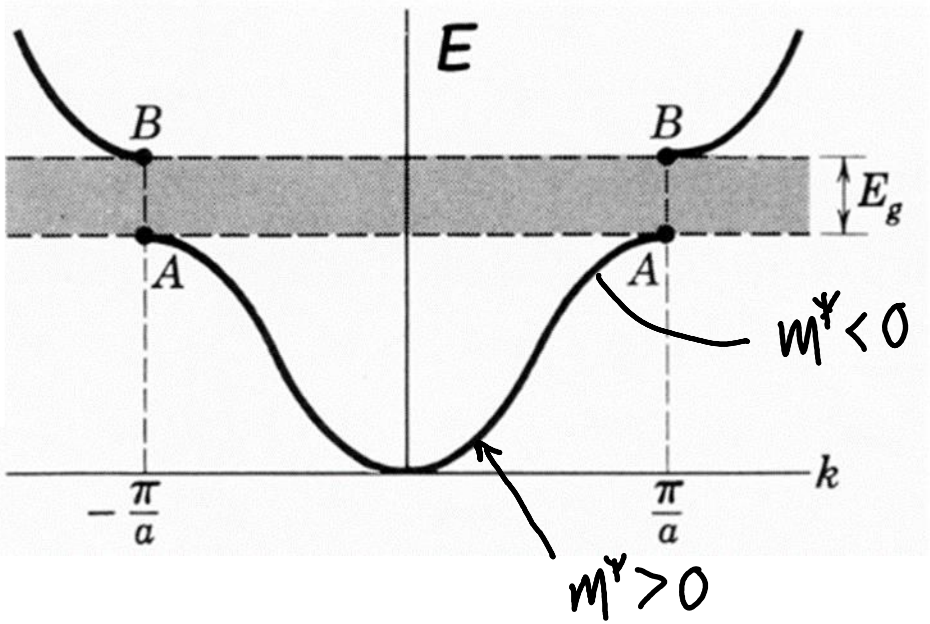
free e- model



$$E(K) = \frac{\hbar^2 K^2}{2m_e} \Rightarrow \frac{d^2E}{dK^2} = \frac{\hbar^2}{m_e} = ct$$

$$m^* = m_e$$

nearly free e- model



$$\bar{K} = (1-\varepsilon)\frac{\bar{G}}{2}$$

$$\bar{K} = \frac{\bar{G}}{2}$$

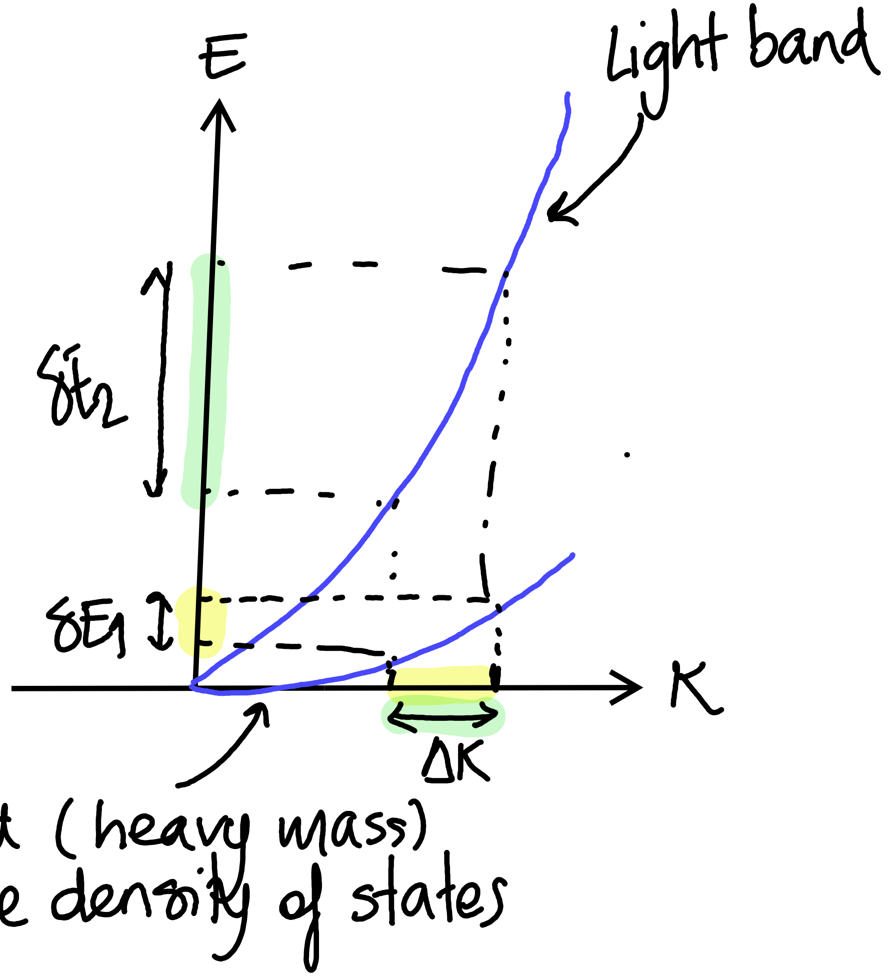
Effective mass and density of states $N(E)$

for free e^-, $E(K)$ is parabolic :

$$N(E) \equiv \frac{dn}{dE} = \frac{dn}{dK}\frac{dK}{dK} = \frac{\sqrt{2}\, m^{3/2}}{\pi^2 \hbar^3} E^{1/2}$$

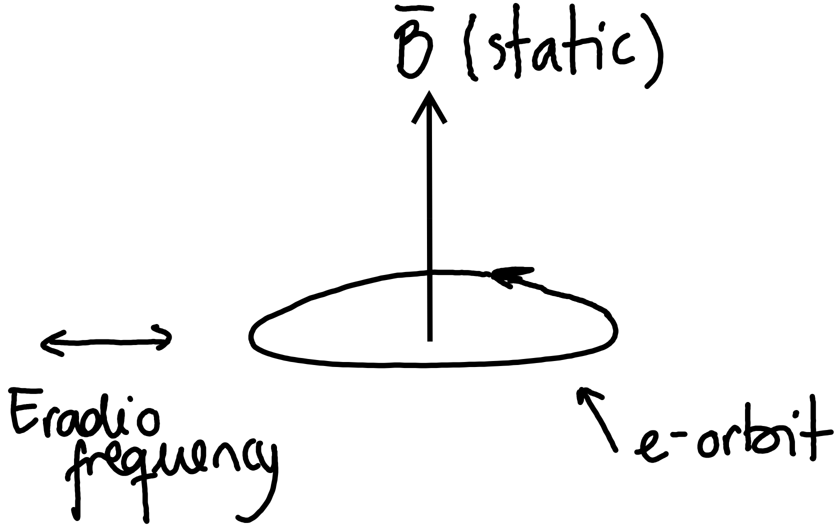
Locally, close to an energy E_0 where $E(K)$ is parabolic and isotropic, $N(E)$ can be generalized as:

$$N(E) = \frac{2^{1/2} m^{*3/2}}{\pi^2 \hbar^3} (E - E_0)^{1/2}$$



How to measure the effective mass?

Cyclotron ressonance



the system absorbs energy when

$$\omega = \omega_c = \frac{eB}{m^*}$$

↑ unknown parameter to be determined.

Summary of the properties of $\vec{k}$ used in the Bloch functions

* Is $\hbar\vec{k}$ the physical momentum of the electron? No

It is a quantum number describing the e- state within a band.
Each band is labelled using index j

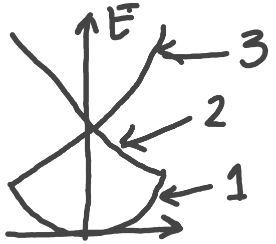
* For each j, which values does $\vec{\mathbf{k}}$ take?

All values consistent with Born-von-Karman boundary conditions within the 1st B.Z (in notation used, $\bar{K}$ runs through all $\bar{q}$)
j runs over an ∞-number of discrete values

* Does the electronic dispersion relationship $E_j(\vec{k})$ have an explicit form? - No

the only constraint to $E(K)$ is that it must be periodic $E_j(\bar{K}) = E_j(\bar{K}+\bar{G})$

* velocity of an e- with energy $E_j(\bar{K})$ is $\bar{v} = \frac{1}{\hbar}\nabla_{\bar{K}} E_j(\bar{K})$
* the rate of change of $\bar{K}$ under an external force is $\hbar\frac{d\bar{K}}{dt} = \bar{f}$
* the electronic wavefunction is $\psi(\bar{r}) = e^{i\bar{K}\bar{r}} u_{j,\bar{K}}(\bar{r})$



K specifies an e- state (or orbital with energy $E_j(K)$ (or $= E_n(K)$))

$\psi_{j\bar{K}}(\bar{r})$: For each j (n), the set of electronic levels $E_j(\bar{K})$ is an <u>energy band</u>

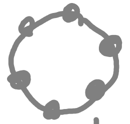
j = band index (in some books: "n")

Reminder

$$\psi(\bar{r}) = \sum_K c_K e^{iKr}$$

Periodic boundary conditions

$$\psi(\bar{r} + N_j a_j) = \psi(\bar{r})$$



$$\bar{K}\cdot a_j = 2\pi \frac{m_j}{N_j}$$ ← integer

in 1D $K = \frac{2\pi}{a}\frac{m}{N}$

in 3D $K = \sum_{i=1}^{3} \frac{m_i}{N_i}\vec{b_i}$