PHYS 460 - LECTURE 14

SEMICONDUCTORS

PERHAPS THE GREATEST IMPACT OF CONDENSED MATTER PHYSICS (AT LEAST IN THE 20th CENTURY) IS THE RISE OF THE SEMICONDUCTOR INDUSTRY AND ASSOCIATED TECHNOLOGIES (DIODES, SOLAR CELLS, TRANSISTORS!) THIS ENTIRE INDUSTRY IS ASSOCIATED WITH THE UNDERSTANDING AND CONTROL OF MATERIAL PROPERTIES, USING MANY OF THE IDEAS WE HAVE BEEN DISCUSSING IN THIS COURSE. WE WILL NOW DISCUSS MANY OF THESE IDEAS, AND INTRODUCE SEVERAL MORE, IN THE CONTEXT OF SEMICONDUCTORS.

WHAT IS A SEMICONDUCTOR?

EXPERIMENTALLY, MATERIALS ARE CLASSIFIED AS SEMICONDUCTORS BASED ON THE MAGNITUDE AND TEMPERATURE DEPENCE OF CONDUCTIVITY

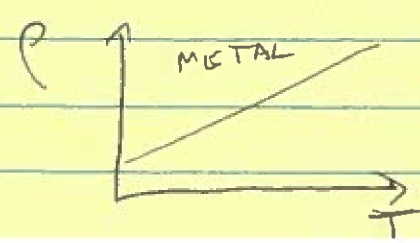
MAGNITUDE: $\rho = \frac{1}{\sigma} \sim 10^{-2} - 10^{9}\ \Omega\text{-cm}$

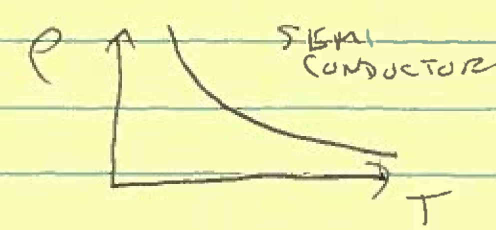
T-DEPENDENCE: RECALL $\sigma = \frac{ne^2\tau}{m}$

IN METALS, $n = \text{const}$, $\tau \propto T$ at high-T

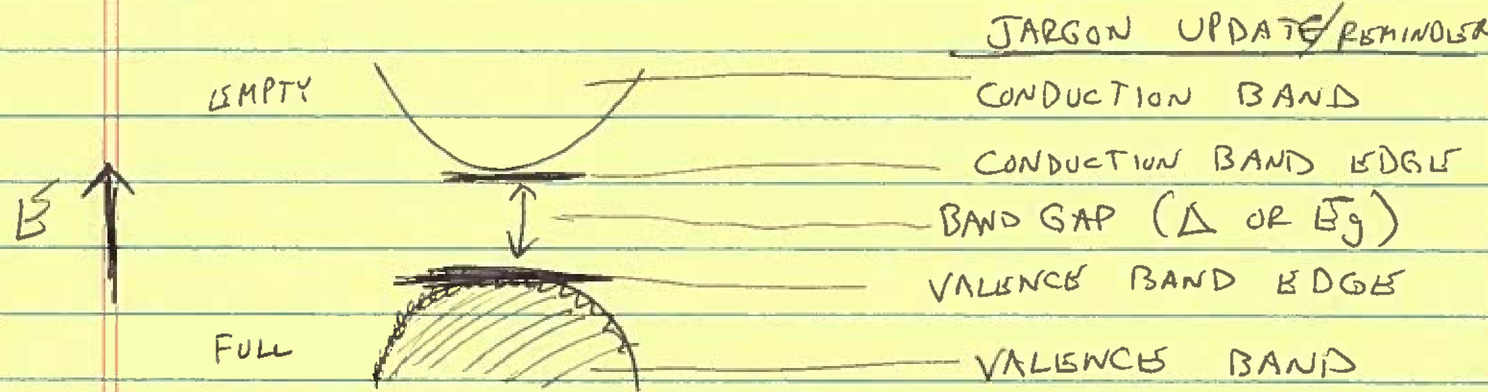
IN SEMICONDUCTORS, $n \propto e^{-\text{const}/T}$

QUALITATIVELY DIFFERENT!





MICROSCOPICALLY, I'VE ALREADY POINTED OUT, SEMICONDUCTORS ARE ACTUALLY INSULATORS AT $T = 0K$, BUT WHOSE BAND GAPS ARE NARROW ENOUGH THAT CHARGE CARRIERS ARE THERMALLY EXCITED ACROSS THE GAP AT ACCESSIBLE TEMPERATURES



WELL KNOWN EXAMPLES:

Si, Ge — "DIAMOND TYPE", BECAUSE OF LATTICE TYPES (SAME AS DIAMOND)

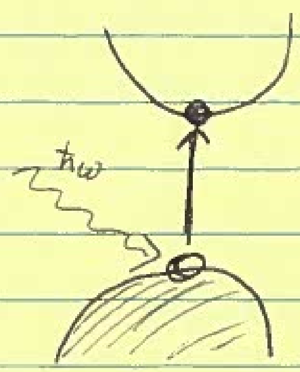
GaAs, InSb — III-V COMPOUNDS — BECAUSE OF COLUMNS IN PERIODIC TABLE (AND VALENCE)

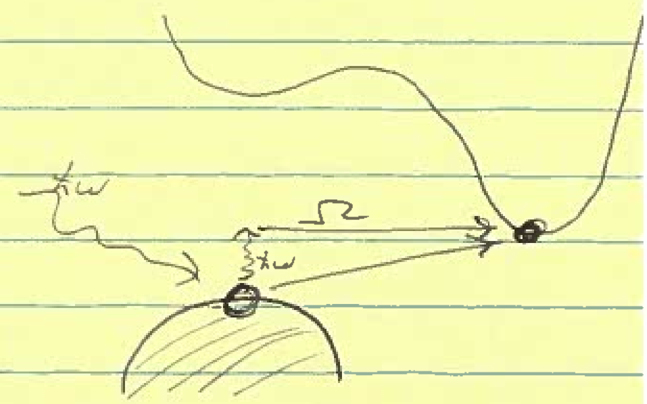
ZnS_2, CdS_2 — II-VI COMPOUNDS FOR SIMILAR REASONS

SIMONS DEFINES SEMICONDUCTOR IF $\Delta < 4eV$. MORE TYPICALLY, $\Delta_{Si} \approx 1eV$, $\Delta_{Ge} \approx 0.8eV$

WE WILL SEE $\rightarrow n \propto e^{\frac{-\Delta}{2k_BT}} \approx 10^{-17} \rightarrow$ OBSERVABLE! (RECALL $N_A = 6.02\times10^{23}$)

BAND GAPS ARE MEASURED VIA OPTICAL ABSORPTION EXPERIMENTS. THIS ITSELF REVEALS TWO CATEGORIES OF SEMICONDUCTORS





"DIRECT" BAND GAP

$\vec{k}_f \approx \vec{k}_i \quad (\vec{k}_\gamma \approx 0)$

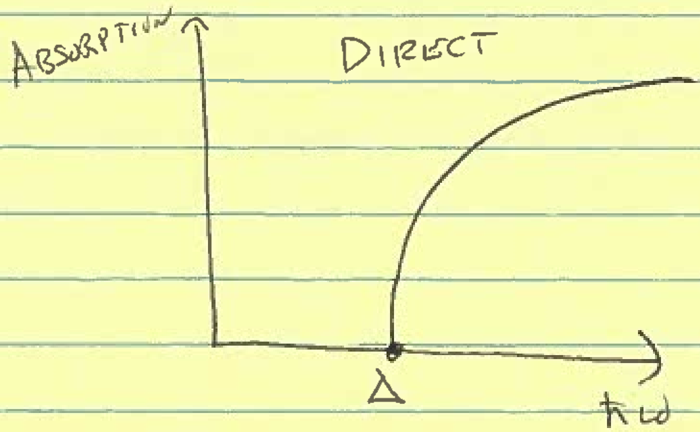
$\Delta = \hbar\omega$

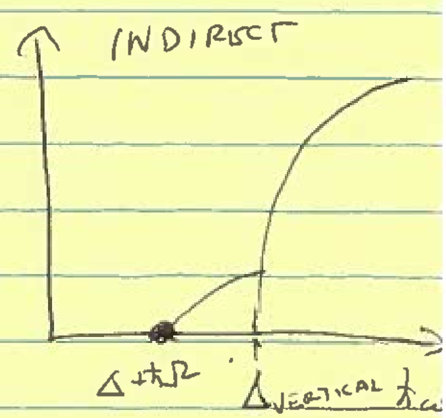
BY CONSERVATION OF ENERGY

"INDIRECT BAND GAP"

TO CONSERVE (CRYSTAL) MOMENTUM ELECTRON MUST BE GIVEN ENERGY FROM PHOTON <u>AND</u> GET MOMENTUM BY SCATTERING OFF A PHONON

AGAIN, CAN SEE IN EXPERIMENT





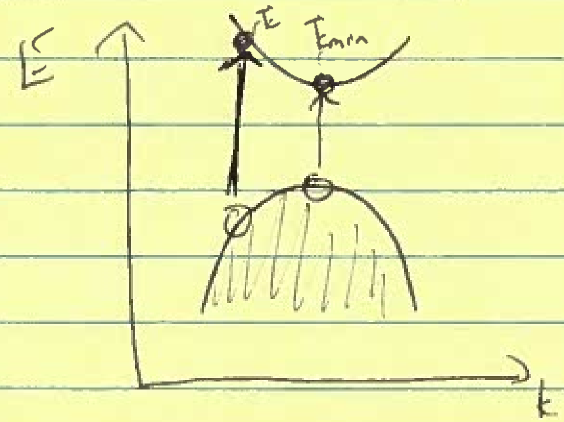
INDIRECT TRANSITIONS ARE MORE COMPLEX AND THEREFORE LESS LIKELY → SCATTERING WEAKER.

OFTEN SEE INDIRECT AND THEN DIRECT (VERTICAL) GAPS

ELECTRONS AND "HOLES"

NOW LET'S LOOK AT WHAT HAPPENS WHEN AN ELECTRON IS PROMOTED FROM THE VALENCE TO THE CONDUCTION BAND (EITHER BY A PHOTON OR BY THERMAL FLUCTUATION)

FOR NOW, LET'S RESTRICT OUR ATTENTION TO DIRECT BAND GAP SEMICONDUCTORS AND LOOK AT THE BANDS NEAR THE BZ BOUNDARY (WHERE THE GAP OPENS UP). WHEN WE WERE STUDYING BAND THEORY, WE SAW BANDS NEAR THE GAP ALWAYS LOOKED LIKE



WITH QUADRATIC DISPERSION. THAT IS, ONCE PROMOTED TO THE CONDUCTION BAND, THE ENERGY OF THE ELECTRON IS GIVEN BY

$$E_{\vec{k}} = E_{min} + \alpha\,|\vec{k}-\vec{k}_{min}|^2$$

ASSUMING AN ISOTROPIC BAND, AND $\alpha > 0$

WE HAVE NOTED BEFORE THAT QUADRATIC DISPERSION IS REMINISCIENT OF FREE ELECTRONS

$$E_{free} = \frac{\hbar^2 k^2}{2m}$$

LEADING TO THE DEFINITION OF "EFFECTIVE MASS" IN THE CONDUCTION BAND

$$m^* \equiv \frac{\hbar^2}{2\alpha} \quad \text{OR} \quad \boxed{\frac{1}{m^*} \equiv \frac{1}{\hbar^2}\frac{\partial^2 E}{\partial k^2}}$$

OR MORE GENERALLY, IN THE CASE OF ANISOTROPIC BANDS, ONE DEFINES AN EFFECTIVE MASS TENSOR

$$\boxed{\left(\frac{1}{m^*}\right)_{\mu\nu} = \frac{1}{\hbar^2}\frac{d^2E}{dk_\mu dk_\nu}}$$

WHICH QUANTIFIES HOW MUCH MORE MASSIVE (AND THUS DIFFICULT TO MOVE) ELECTRON ARE WHEN TRAVELLING IN DIFFERENT DIRECTIONS

PUSHING THE ANALOGY WITH FREE ELECTRONS FURTHER, WE CAN ALSO ASSOCIATION THE (GROUP) VELOCITY OF THE ELECTRON WITH THE GRADIENT OF ENERGY

$$\boxed{\vec{v}_e = \frac{1}{\hbar}\vec{\nabla}_k E = \frac{\hbar}{m^*}(\vec{k}-\vec{k}_{min})}$$

OKAY... BUT DOES THIS MAKE SENSE? CAN WE REALLY RELATE EFFECTIVE MASS, AS DEFINED BY BAND DISPERSION, TO INERTIAL MASS IN NEWTON'S SECOND LAW?

YES, AS IT TURNS OUT!

APPLY FORCE, $\vec{F}$, THEN WORK PER UNIT TIME

$$\frac{dW}{dt} = \vec{F}\cdot\vec{v} = \frac{1}{\hbar}\vec{F}\cdot\vec{\nabla}_k E$$

BUT ALSO $\quad \frac{dE}{dt} = \frac{d\vec{k}}{dt}\cdot\vec{\nabla}_k E \quad$ (CHAIN RULE)

$$\Rightarrow \boxed{\vec{F} = \hbar\frac{d\vec{k}}{dt} = \frac{d\vec{p}}{dt}}$$ NEWTON'S SECOND LAW

OR USING $\vec{v} = \frac{\hbar}{m^*}(\vec{k} - \vec{k}_{min})$

$$\boxed{\vec{F} = m^* \frac{d\vec{v}}{dt}}$$

AWESOME! WHAT IS $\vec{F}$? OBVIOUS APPLICATIONS ARE QUANTIFYING RESPONSE TO (WEAK) ELECTRIC AND MAGNETIC FIELDS. IN FACT, SINCE THE DENSITY OF ELECTRONS IN THE CONDUCTION BAND IS SO LOW, WE CAN FORGET ABOUT THE EFFECTS OF PAULI EXCLUSION (WE WILL RETURN TO THIS) AND SIMPLY APPLY THE <u>DRUDE MODEL</u> TO DESCRIBE ELECTRON MOTION

$$\boxed{m_e^* \frac{d\vec{v}}{dt} = -e(\vec{E} + \vec{v} \times \vec{B}) - \frac{m_e^* \vec{v}}{\tau}}$$

RELAXATION TIME

THIS IS COMMONLY REFERRED TO AS THE ELECTRON "EQUATION OF MOTION"

τ IS "SCATTERING TIME" OR "RELAXATION TIME" AND IS CLOSELY CONNECTED TO ANOTHER PARAMETER OF COMMON INTEREST — THE ELECTRON "MOBILITY", μ_e,

$$\mu_e = \frac{|\vec{v}|}{|\vec{E}|} = \left|\frac{e\tau}{m^*}\right|$$

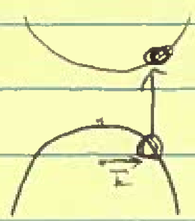
WHICH QUANTIFIES HOW EASILY ELECTRONS MOVE.

BUT ELECTRONS ARE NOT THE WHOLE STORY!
WHEN THE ELECTRON AT STATE, $\vec{k}$, WAS PROMOTED TO THE CONDUCTANCE BAND, IT LEFT AN <u>EMPTY ORBITAL</u> IN THE VALENCE BAND.

THIS EMPTY ORBITAL IS CALLED A "<u>HOLE</u>", AN ITSELF CAN CARRY CURRENT BY FACILITATING MOTION OF ELECTRONS IN NEAR-FULL BAND. INSTEAD OF TRACKING THE $N-1$ FULL ELECTRON STATES, IT IS SIMPLER JUST TO TALK ABOUT 1 EMPTY STATE A $\vec{k}$ - THE HOLE. ~~EMPTY STATE~~ THE DISPERSION OF THE VALENCE BAND NEAR THE MAXIMUM IS GIVEN BY

$$E = E_{max} - \alpha \left|\vec{k} - \vec{k}_{max}\right|^2$$

$$\alpha > 0$$



IN MODERN PARLANCE (BUT NOT ALWAYS IN THE PAST), THE CONVENTION IS TO DEFINE A <u>POSITIVE</u> HOLE EFFECTIVE MASS, ANALOGOUS TO ELECTRONS

$$\boxed{\frac{1}{m_h^*} = \frac{2\alpha}{\hbar^2} = -\frac{1}{\hbar^2}\frac{\partial^2 E}{\partial k^2}}$$

WE THEN CAN DEFINE A POSITIVE ENERGY DISPERSION FOR THE HOLES, USING THE FACT THAT A FULL SHELL HAS ZERO EFFECTIVE ENERGY

$$\boxed{E_{hole} = E_{\substack{FULL\\BAND}} - E_{electron} = \text{Const} + \frac{\hbar^2\left|\vec{k} - \vec{k}_{max}\right|^2}{2m_h^*}}$$

IT IS SOMETIMES CONFUSING THAT INCREASING $\vec{k}$ MAKES HOLE ENERGY INCREASE. JUST REMEMBER, IF HOLE ENERGY GOES DOWN THAT MEANS OTHER ELECTRON ENERGIES ARE FORCED TO INCREASE

SIMILARLY, SINCE

$$\sum_{\text{FULL BAND}}' \vec{k}_i = 0$$

THEN
$$\boxed{\begin{aligned}\vec{k}_{hole} &= \sum_{\text{FULL BAND}}' \vec{k}_i - \vec{k}_{\substack{missing \\ electron}} \\ &= -\vec{k}_{electron}\end{aligned}}$$

$\Rightarrow$ IF WE DEFINE

$$\boxed{\vec{v}_{hole} = \frac{\vec{\nabla}_{\vec{k}_{hole}} E_{hole}}{\hbar} = \vec{v}_{\substack{missing \\ electron}}}$$

AND USING SAME REASONING, THE HOLE EQUATION OF MOTION IS GIVEN BY

$$\boxed{m_h^d \frac{d\vec{v}}{dt} = e\left(\vec{E} + \vec{v}\times\vec{B}\right) - \frac{m_h^\tau \vec{v}}{\tau}}$$

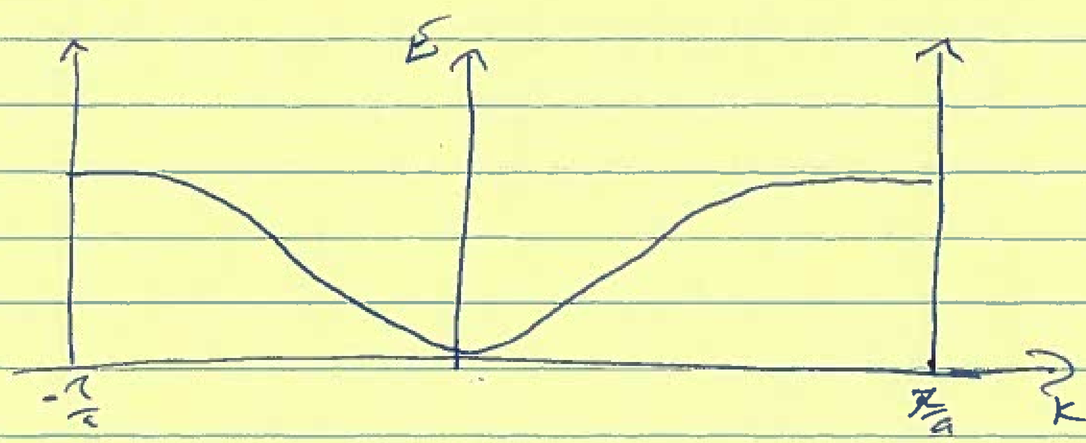
NOTE e POSITIVE! THIS AGAIN REMINDS ~~US~~ US OF MEASURED HALL CONSTANTS, R_H, WITH THE WRONG SIGN (AND IN FACT EXPLAINS THEM.)

SIDEBAR: RELATING EFFECTIVE MASS TO BANDWIDTH

RECALL THAT IN THE 1D TIGHT BINDING CHAIN

$$\varepsilon_k = \varepsilon_0 - 2t\cos ka$$

EARLIER I POINTED OUT THAT THIS DISPERSION IS QUADRATIC AS $ka \to 0$, AND INTRODUCED THE CONCEPT OF EFFECTIVE MASS THEN FROM OUR RECENT DISCUSSION, HOWEVER, IT IS CLEAR THAT WE SHOULD BE EXPANDING ABOUT THE MAXIMUM NEAR THE ZONE BOUNDARY, WHICH GIVES A QUADRATIC HOLE BAND



AT BZ BOUNDARY $k_{max} = \frac{\pi}{a}$. LET

$$k = \frac{\pi}{a} - q \quad , \text{ WITH } \quad qa \ll 1$$

$$\Rightarrow \quad \varepsilon_k = \varepsilon_0 - 2t\left(-1 + \frac{q^2a^2}{2}\right)$$

$$= \varepsilon_0 + 2t - t a^2 q^2$$

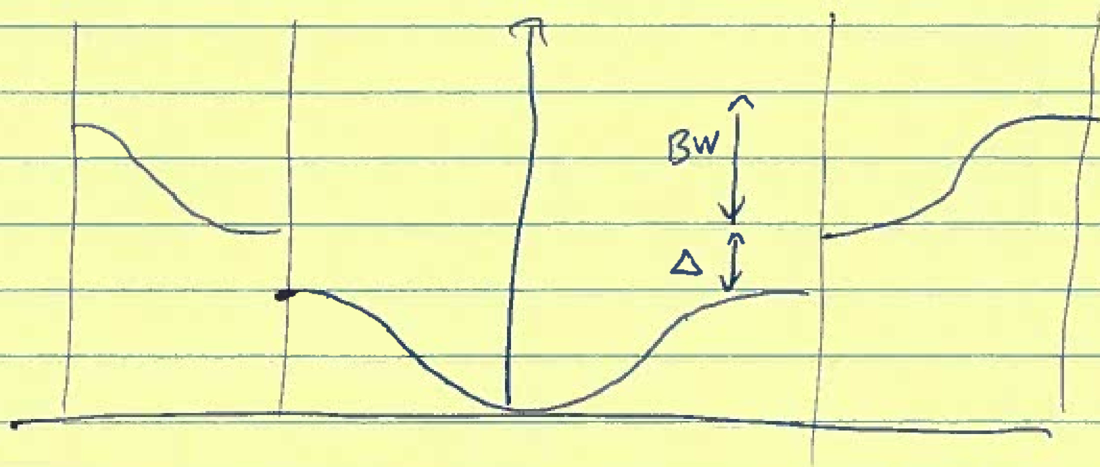
So $\dfrac{1}{m_h^*} = -\dfrac{1}{\hbar^2}\dfrac{\partial^2 E}{\partial k^2} = \dfrac{1}{\hbar^2}2ta^2$

$$\boxed{m_h^* = \frac{\hbar^2}{2ta^2}}$$

SO EFFECTIVE DECREASES (ELECTRONS MOVE MORE EASILY) AS HOPPING PARAMETER INCREASES. THIS MAKES SENSE.

THIS ALSO MEANS THAT <u>EFFECTIVE MASS DECREASES AS BANDWIDTH INCREASES</u>. THIS IS GENERALLY TRUE.

YOU SEE IT IN THE NEARLY FREE ELECTRON PICTURE TOO.



BIGGER GAP (STRONGER LATTICE INTERACTION) → SMALL BANDWIDTH → FLATTER BANDS → LARGER EFFECTIVE MASS.

<u>GAP SIZE IS ALSO AN INDICATOR OF EFFECTIVE MASS!</u>