PHYS 460 LECTURE 15

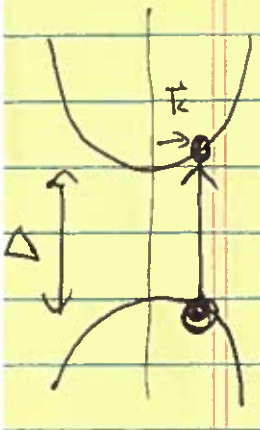
SEMICONDUCTORS, CONTINUED...

LAST LECTURES, WE WERE DISCUSSING SEMICONDUCTORS AS SMALL BAND-GAP INSULATORS, AND IN PARTICULAR THE TYPES OF CHARGE CARRIERS WHICH CAN BE EXCITED IN THESE SYSTEMS, EITHER BY LIGHT OR THERMAL FLUCTUATIONS.

WE FOUND THAT THERE WERE TWO TYPES:

ELECTRONS

OCCUPIED STATES NEAR BOTTOM OF (NEARLY) EMPTY CONDUCTION BAND



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

$$m_e^* = \frac{\hbar^2}{\frac{\partial^2 E}{\partial k^2}} = \frac{\hbar^2}{2\alpha}$$

EFFECTIVE MASS

$$\vec{v}_e = \frac{1}{\hbar} \vec{\nabla}_k E$$

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

HOLES

EMPTY STATES NEAR TOP OF (NEARLY) FULL VALENCE BAND

$$E_e = E_{max} - \alpha |\vec{k} - \vec{k}_{max}|^2$$

$$\Rightarrow E_h = const + \alpha |\vec{k} - \vec{k}_{max}|^2$$

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

$$\vec{k}_{hole} = -\vec{k}_e$$

$$\vec{v}_h = \vec{\nabla}_{k_{hole}} E_h = \vec{v}_e$$

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

NOTE: ALWAYS BEAR IN MIND ALTERNATE DEF OF m_h^* WHICH IS -VE!

STATISTICAL MECHANICS OF ELECTRONS/HOLES

SEMICONDUCTORS ARE SPECIAL BECAUSE THEIR BAND GAPS ARE SMALL ENOUGH THAT THERMAL FLUCTUATIONS CAN EXCITE A SMALL NUMBER OF CARRIERS AT ACCESSIBLE TEMPERATURES ($T \sim 300K$). WE KNOW HOW TO CALCULATE THE CARRIER DENSITY FROM OUR PREVIOUS EXPERIENCE WITH FREE ELECTRONS (i.e. SOMMERFELD THEORY)

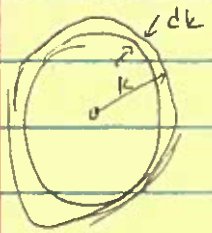
$$n = \frac{N}{V} = \int_0^\infty g(\varepsilon)\, f_{FD}(\varepsilon - \mu)\, d\varepsilon$$

WHERE $f_{FD} = \dfrac{1}{e^{\frac{\varepsilon-\mu}{k_B T}} + 1}$ IS THE FERMI-DIRAC DISTRIB.

AND $g(\varepsilon)$ = DENSITY OF STATES PER UNIT VOLUME

FOR FREE ELECTRONS, RECALL THAT

$$\varepsilon(k) = \frac{\hbar^2 k^2}{2m} \Rightarrow k = \sqrt{\frac{2\varepsilon m}{\hbar^2}}$$



$$g(\varepsilon)d\varepsilon = \frac{2}{(2\pi)^3} 4\pi k^2 dk = \frac{1}{\pi^2}\left(\frac{2\varepsilon m}{\hbar^2}\right)\sqrt{\frac{2m}{\hbar^2}}\,\frac{\varepsilon^{-\frac{1}{2}}}{2}\,d\varepsilon$$

$$= \frac{(2m)^{3/2}}{2\pi^2\hbar^3}\,\varepsilon^{\frac{1}{2}}\,d\varepsilon$$

THROUGH THE SAME REASONING, CONDUCTION ELECTRONS WITH ENERGY

$$\mathcal{E} = \mathcal{E}_c + \frac{\hbar^2 k^2}{2m_e^*}$$

HAVE $$\boxed{g_e(\mathcal{E} > \mathcal{E}_c) = \frac{(2m_e^*)^{3/2}}{2\pi^2\hbar^3}(\mathcal{E} - \mathcal{E}_c)^{1/2}}$$

IF $\mathcal{E}_c - \mu \gg k_B T$ (GAP IS BIG "ENOUGH")

$$f_{FD}^e = \frac{1}{e^{\frac{\mathcal{E}-\mu}{k_B T}} + 1} \approx e^{-\frac{(\mathcal{E}-\mu)}{k_B T}}$$

i.e. FERMI-DIRAC STATISTICS REDUCES TO SIMPLE BOLTZMAN STATISTICS (WHICH WE MIGHT NOTICE JUSTIFY USE OF DRUDE MODEL)

$$\Rightarrow n(T) \approx \frac{(2m_e^*)^{3/2}}{2\pi^2\hbar^3} \int_{\mathcal{E}_c}^{\infty} (\mathcal{E} - \mathcal{E}_c)^{1/2} e^{-\frac{(\mathcal{E}-\mu)}{k_B T}} d\mathcal{E}$$

$$= \frac{(2m_e^*)^{3/2}}{2\pi^2\hbar^3} e^{\frac{\mu - \mathcal{E}_c}{k_B T}} \int_{\mathcal{E}_c}^{\infty} (\mathcal{E} - \mathcal{E}_c)^{1/2} e^{-\frac{(\mathcal{E}-\mathcal{E}_c)}{k_B T}} d\mathcal{E}$$

SUB $x = \mathcal{E} - \mathcal{E}_c$, $y = \sqrt{x}$, $dy = \frac{1}{2} x^{-1/2} dx$

$$\Rightarrow n(T) = \frac{(2m_e^*)^{3/2}}{2\pi^2\hbar^3} e^{\frac{\mu - \mathcal{E}_c}{k_B T}} \int_0^{\infty} x^{1/2} e^{-\frac{x}{k_B T}} dx$$

$$= \frac{(2m_e^*)^{3/2}}{2\pi^2\hbar^3} e^{\frac{\mu - E_c}{k_B T}} \times \frac{1}{2} (k_B T)^{3/2} \sqrt{\pi}$$

AFTER SOME MANIPULATION

$$\Rightarrow \boxed{n(T) = \frac{1}{4} \left(\frac{2 m_e^* k_B T}{\pi \hbar^2} \right)^{3/2} e^{-\frac{(E_c - \mu)}{k_B T}}}$$

WE CAN DO A SIMILAR CALCULATION FOR HOLES AT THE TOP OF THE VALENCE BAND

$$E = E_v - \frac{\hbar^2 k^2}{2 m_h^*}$$

$$\Rightarrow \boxed{g_v(E < E_v) = \frac{(2m_h^*)^{3/2}}{2\pi^2\hbar^3} (E_v - E)^{1/2}}$$

HOLES ARE THE ABSENCE OF ELECTRONS

$$\Rightarrow f_{FD}^h = 1 - f_{FD}^e = 1 - \frac{1}{e^{\frac{(E-\mu)}{k_B T}} + 1}$$

$$= \frac{e^{\frac{(E-\mu)}{k_B T}}}{e^{\frac{E-\mu}{k_B T}} + 1}$$

$$= \frac{1}{e^{\frac{\mu - E}{k_B T}} + 1}$$

IF $\mu - \mathcal{E}_v \gg k_B T$ (AGAIN, μ INSIDE GAP, GAP BIG ENOUGH)

$$f^h \approx e^{\frac{\mathcal{E}-\mu}{k_B T}}$$

$$p(T) = \int_{-\infty}^{\mathcal{E}_v} g_v(\mathcal{E})\, f^h(\mathcal{E}-\mu)\, d\mathcal{E}$$

p for "positive" charges

$$\simeq \int_{-\infty}^{\mathcal{E}_v} g_v(\mathcal{E})\, e^{\frac{\mathcal{E}-\mu}{k_B T}}\, d\mathcal{E}$$

MATH, MATH, MATH

$$\boxed{p(T) = \frac{1}{4}\left(\frac{2 m_h^* k_B T}{\pi \hbar^2}\right)^{3/2} e^{-\frac{(\mu - \mathcal{E}_v)}{k_B T}}}$$

THE GREAT UNKNOWN IN BOTH OF THESE EQUATIONS IS THE CHEMICAL POTENTIAL, $\mu(T)$ HOWEVER THE PRODUCT OF $n(T)$ AND $p(T)$ DOES NOT HAVE THIS ISSUE

$$\boxed{n(T)p(T) = \frac{1}{2}\left(\frac{k_B T}{\pi \hbar^2}\right)^3 \left(m_e^* m_h^*\right)^{3/2} e^{-\frac{(\mathcal{E}_c - \mathcal{E}_v)}{k_B T}}}$$

NOTE $\mathcal{E}_c - \mathcal{E}_v = \Delta$ = GAP

THIS IS KNOWN AS THE SEMICONDUCTOR "LAW OF MASS ACTION" (NAMED AFTER SAME IN CHEMISTRY)

WHEN THE CONDUCTION ELECTRONS ARE ALWAYS THE RESULT OF ELECTRONS EXCITED FROM VALENCE BAND (THE ONLY CASE WE HAVE CONSIDERED SO FAR), WE REFER TO THE MATERIAL AS AN "INTRINSIC SEMICONDUCTOR" AND

$$n(T) = p(T) = \frac{1}{\sqrt{2}} \left(\frac{k_B T}{\pi \hbar^2} \right)^{3/2} \left(m_e^* m_h^* \right)^{3/4} e^{\frac{-\Delta}{2 k_B T}}$$

INTRINSIC SEMICONDUCTOR

NOTE 2 IN EXP

OR TAKING RATIO

$$\frac{n(T)}{p(T)} = 1 = \left(\frac{m_e^*}{m_h^*} \right)^{3/2} e^{\frac{-(\varepsilon_c + \varepsilon_v - 2\mu)}{k_B T}}$$

$$0 = \frac{3}{2} \ln \left(\frac{m_e^*}{m_h^*} \right) - \frac{(\varepsilon_c + \varepsilon_v)}{k_B T} + \frac{2\mu}{k_B T}$$

$$\Rightarrow \mu(T) = \frac{\varepsilon_c + \varepsilon_v}{2} + \frac{3 k_B T}{4} \ln \left(\frac{m_h^*}{m_e^*} \right)$$

INTRINSIC SEMICOND.

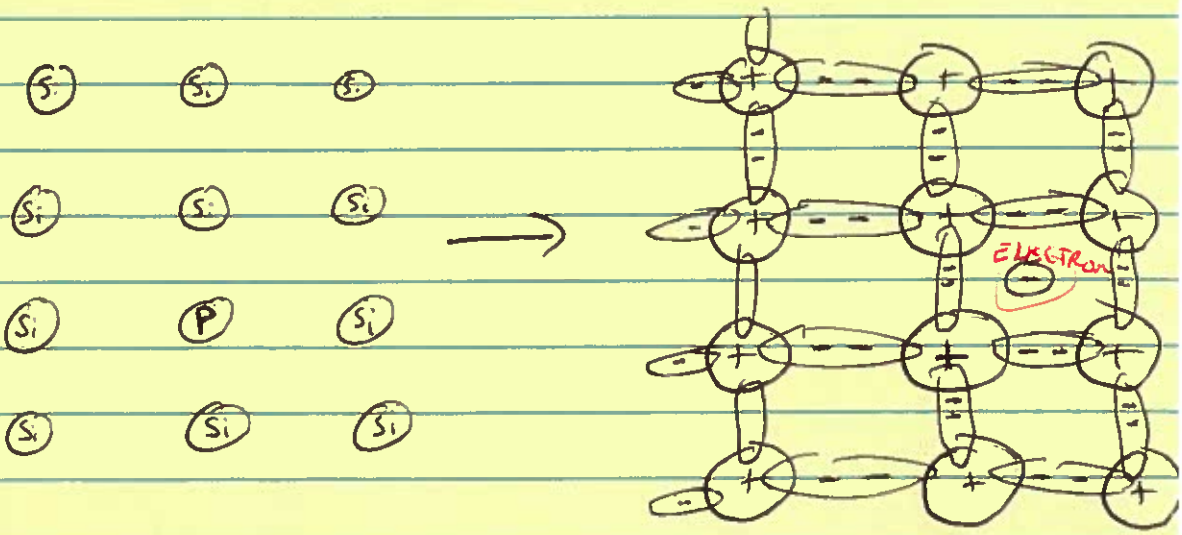
NOTE THAT THIS CONFIRMS THE IDEA THAT μ LIES INSIDE THE GAP.

AT $T = 0$, μ IS PRECISELY MID-GAP, AND IF $m_h^* = m_e^*$, IT IS ALWAYS MID-GAP (FOR INTRINSIC SEMICONDUCTORS)

OK, BUT WHY DID I MAKE A POINT OF SAYING THAT THESE FORMULAS (ON THE LAST PAGE) ARE FOR "INTRINSIC" SEMICONDUCTORS? WHEN ARE SEMICONDUCTORS NOT INTRINSIC? ANSWER: WHEN THE CARRIERS ARE THE RESULT OF IMPURITIES IN THE CRYSTALS. IN THIS CASE, THE SEMICONDUCTORS (OR CARRIERS) ARE "EXTRINSIC" SEMICONDUCTORS

HOW DOES THIS WORK?

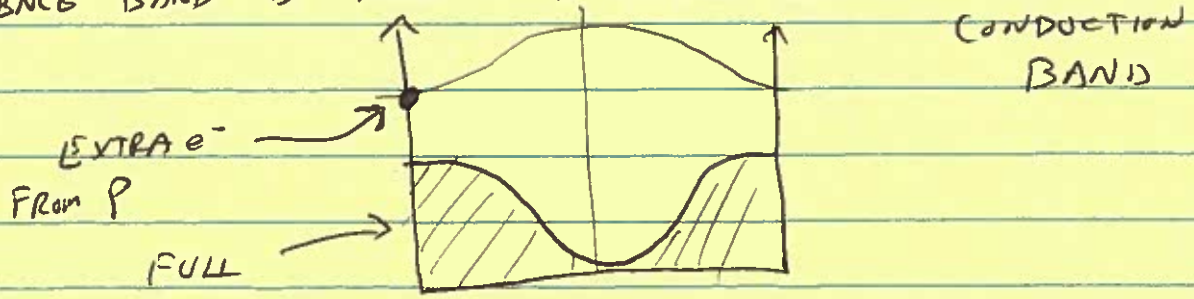
CLASSIC EXAMPLE: LONE P ATOM INSIDE Si CRYSTAL



Si IS A TETRAVALENT ATOM, AND THE CRYSTAL IS STABILIZED BY 4-COVALENT BONDS AROUND EACH ATOM → DIAMOND STRUCTURE

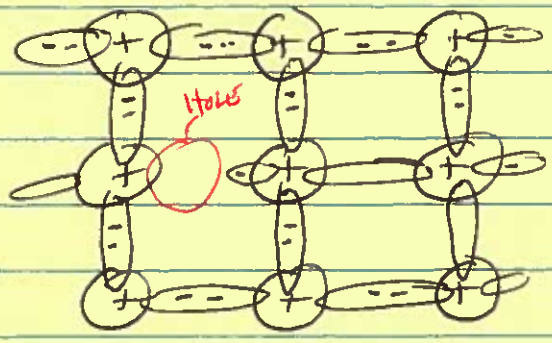
P HAS ONE EXTRA ELECTRON, SO EVEN ONCE ALL BONDS ARE SATISFIED, THERE IS AN EXTRA ELECTRON FREE TO HOP AROUND.

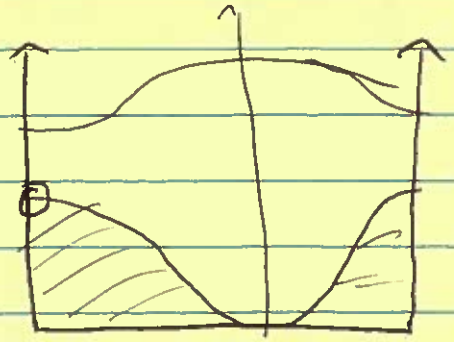
OR, IN BAND LANGUAGE, A Si CRYSTAL WITH A P IMPURITY IS THE SAME AS Si WITH ONE EXTRA ELECTRON (AND PROTON). BUT THE VALENCE BAND IS FULL → EXTRA ELECTRON GOES TO CONDUCTION BAND



IN THIS SCENARIO, P IS KNOWN AS AN "n-DOPANT" OR ELECTRON "DONOR"

AS YOU MIGHT ANTICIPATE, YOU CAN ALSO MANIPULATE THE MATERIAL IN THE OPPOSITE WAY IF ONE INSTEAD SUBSTITUTES ONE Si ATOM WITH AN ATOM OF Al (OR B), THERE WILL BE ONE FEWER ELECTRONS





THIS IS THE SAME AS ADDING ONE HOLE TO THE VALENCE BAND

FOR THIS REASON, ATOMS LIKE Al (IN THE CASE OF Si) ARE KNOWN AS "p-DOPANTS" OR ELECTRON "ACCEPTOR"

BUT HOLD ON: THESE IMPURITY ATOMS ALSO CHANGE THE NUMBER OF PROTONS. DOESN'T THAT CHANGE THINGS? WELL, YES AND NO.

CONSIDER THE CASE OF A P (n-dopant) ATOM IN Si. THE n-DOPANT ADDED 1 ELECTRON AND 1 PROTON. THE PROTON CREATES AN EXCESS POSITIVE CHARGE IN THE LATTICE STRUCTURE WHICH CAN BIND FREE ELECTRONS THE POTENTIAL BETWEEN AN ELECTRON AND THIS EXCESS PROTON IS GIVEN BY

$$V = \frac{e^2}{4\pi\varepsilon_0 \varepsilon_r r}$$

WHERE r IS THE DISTANCE BETWEEN THE TWO PARTICLES AND ε_r IS THE RELATIVE DIELECTRIC CONSTANT, WHICH ACCOUNTS FOR HOW WELL THE SEA OF ELECTRONS SCREEN THE POSITIVE CHARGE

THIS IS JUST A MODIFIED FORM OF THE HYDROGEN ATOM PROBLEM. RECALL, FOR HYDROGEN, ENERGIES WERE GIVEN BY

$$E_n^{\text{HYDROGEN}} = -\frac{R_y}{n^2}$$

WHERE $$R_y = \frac{me^2}{8\varepsilon_0^2 h^2} \approx 13.6\,eV$$

WAS THE RYDBERG CONSTANT

ALSO, FOR HYDROGEN, THE ORBITAL RADIUS WAS GIVEN BY

$$r_n \approx n^2 a_0$$

WHERE $a_0 = \frac{4\pi\varepsilon_0 \hbar^2}{m e^2} \approx 0.51 \times 10^{-10}\ m$

WAS THE BOHR RADIUS.

IN THE CASE OF P IN Si, WE CAN DO THE EXACT SAME CALCULATION (IF WE WERE SO INCLINED) WITH THE MODIFICATIONS $\varepsilon_0 \longrightarrow \varepsilon_0 \varepsilon_r$ AND $m \longrightarrow m_e^*$

$$\rightarrow \quad E \sim R_y^{eff} = R_y \times \left(\frac{m_e^*}{m}\right) \times \left(\frac{1}{\varepsilon_r}\right)^2$$

$$\text{AND} \quad r \sim a_0^{eff} = a_0 \times \left(\frac{m}{m_e^*}\right) \times (\varepsilon_r)$$

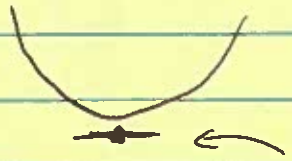
CLEARLY, THESE VALUES DEPEND ON THE SPECIFIC MATERIAL, BUT FOR Si (WHICH IS TYPICAL)

$$\frac{m_e^*}{m} \sim 0.2 \quad \text{AND} \quad \varepsilon_r \sim 12$$

$$\Rightarrow a_0^{eff} = \frac{(0.5\text{Å})}{0.2} \times 12 = 30\text{Å}$$

$$R_y^{eff} = 13.6\text{eV} \times 0.2 \times \frac{1}{12^2} \approx 0.02\text{eV}$$

THIS MEANS THAT THERE EXISTS A BOUND STATE WITH ENERGIES $\sim 0.02\,eV$ BELOW E_c, WHICH ALREADY PARTIALLY DELOCALIZED



AT T=0K, THIS LONELY ELECTRON IS BOUND AND CANNOT CARRY CURRENT (UNLESS THE DENSITY OF DONOR ATOMS IS LARGE ENOUGH TO FORM A "DONOR BAND")

HOWEVER, THE SMALL ENERGY OF R_y^{eff} MEANS THAT ELECTRONS CAN BE THERMALLY EXCITED INTO THE CONDUCTION BAND A TEMPERATURES $T \sim 200K$. AT HIGH TEMPERATURES, YOU GOT A NET EXCESS OF ELECTRONS. AT LOW TEMPERATURES, THESE ELECTRONS "FREEZE OUT"

SIMILAR ARGUMENTS ESTABLISH THE EXISTENCE OF "ACCEPTOR BANDS" (WHOSE NAME NOW MAKES SENSE) WHICH CAN STEAL ELECTRONS AND FORM HOLES AT MODERATES TEMPERATURES