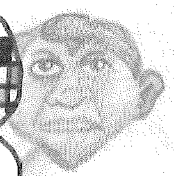
Solids

Rose-Hulman Institute of Technology (1972)
Texas Tech University (1975)
R.J. Marks II Class Notes
(1975)

	1 7:45	2 8:45	3 9:40	4 10:35	5 11:30	6 12:25	7 1:20	8 2:15	9 3:10
MON		SOLIDS A202			MUSIC F203				
TUES		SOLIDS A202							
WED		SOLIDS A202			MUSIC F203		EE LAB II D101	EE LAB II D101	
THUR	PROJECT G219				MUSIC F203				
FRI		SOLIDS A·202	PRO D·202	JECT	MUSIC F203				



3-14-72 (TUES)

AZAROFF & BROPHY "ELECTRONIC PROCESSES", CHAPT 3

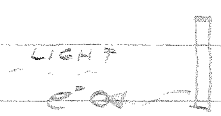
TIPLER "MODERN PHYSICS" SEC 3-4, 5-1, 5-2, 5-5, 5-6, 5-7, 5-8, PP 225-3

COURSE OUTLINE

- CRYSTAL STRUCTURE
- LATTICE VIBRATIONS, THERMAL PROPERTIES
- DIELECTRICS
- MAGNETIC PROPERTIES
- ELECTRICAL CONDUCTION
  - FREE ELECTRON THEORY METALS
  - BAND THEORY - METALS, SEMICONDUCTORS, INSULATORS

LIGHT - WAVE (SO THOUGHT)

PHOTOELECTRIC EFFECT



SHOWED PARTICAL PROPERTY OF LIGHT

PARTICLE (PHOTON)
WAVE (ELECTROMAGNETIC) } DUAL NATURE OF LIGHT

$E = hf$

E = ENERGY

h = PLANCK'S CONSTANT

f = FREQUENCY

$p = h/\lambda = \hbar k$

p = MOMENTUM

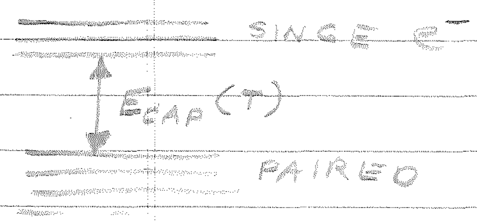
$\hbar = h/2\pi$

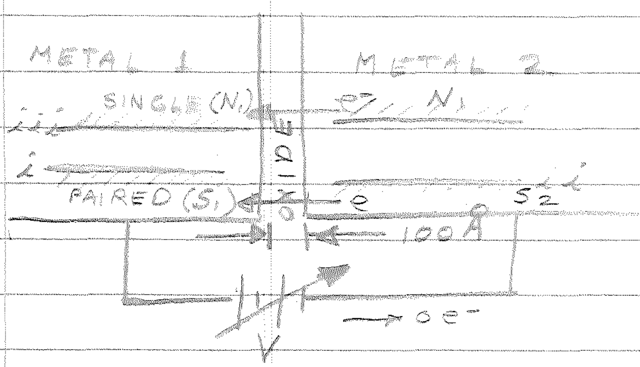
$k = 2\pi/\lambda$

λ = WAVELENGTH

$\vec{k}$ IS IN DIRECTION OF MOTION OF WAVE

HIGH FREQ $\Leftrightarrow$ HIGH ENERGY





WILL HAVE TUNNELING

INCREASING V LIFTS ENERGY OF ELECTRONS ON THE RIGHT (LIFTING ENTIRE RIGHT PICTURE)

ii OPPOSITE GAP ON OTHER SIDE

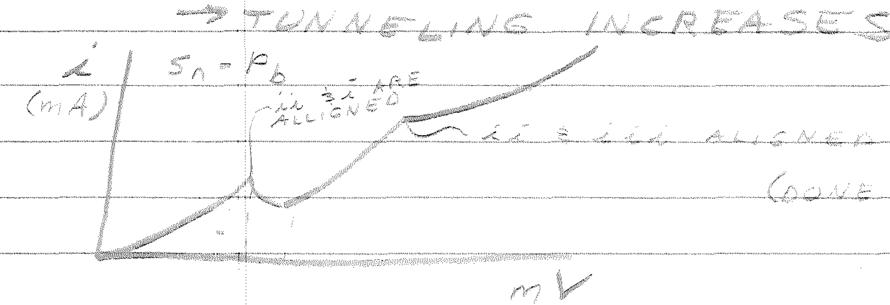
ELECTRONS NEAR ii ARE STOPPED

→ NO STATES ON LEFT AT SOME E_1

INCREASE V FURTHER

WHEN ii IS OPPOSITE iii

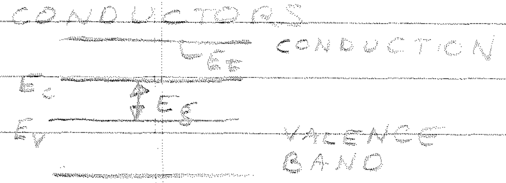
→ TUNNELING INCREASES



(DONE BY GIAEVER)

5-15-73 MON (377-407)

SEMICONDUCTORS

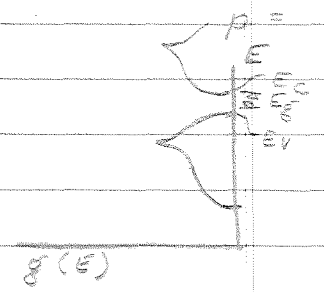


@ $T = 0°K$, ALL VALENCE BAND STATES OCCUPIED BY e^-

$\sigma = n e \mu = 0$, FOR n = FREE e^- = 0 (METALS)

FOR SEMICONDUCTORS

$\sigma = n e \mu_e + p e \mu_h$



p = HOLES/VOLUME, $n = e^-/\text{VOLUME}$

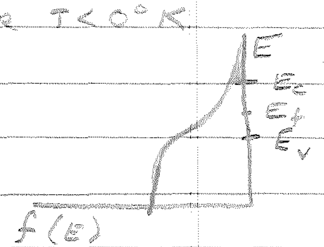
ELECTRONS NEAR THE BOTTOM OF THE CONDUCTION BAND

$$g(E) = \frac{1}{2\pi^2}\left(\frac{2m_e^*}{\hbar^2}\right)^{3/2}(E-E_c)^{1/2}$$

FOR HOLES NEAR TOP OF VALENCE BAND

$$g(E) = \frac{1}{2\pi^2}\left(\frac{2m_h^*}{\hbar^2}\right)^{3/2}(E_v-E)^{1/2}$$

FOR $T<0°K$



E_f = FERMI ENERGY

$E_v < E_f < E_c$

n = NUMBER OF e IN CONDUCTION BAND

$$n = \int_{E_c}^{E_t} g(E)\, f(E)\, dE$$

$$= \frac{1}{2\pi^2}\left(\frac{2m_e^*}{\hbar^2}\right)^{3/2} \int_{E_c}^{\infty} \frac{(E-E_c)^{\frac{1}{2}}\, dE}{e^{(E-E_f)/kT}+1}$$

CLOSE ENOUGH

IF $E_c - E_f \geq 4kT \Rightarrow e^{(E_f-E)/kT}+1 \simeq e^{(E-E_f)/kT}$

$$\Rightarrow n = \frac{1}{2\pi^2}\left(\frac{2m_e^*}{\hbar^2}\right)^{3/2}(kT)^{3/2} e^{(E_f-E_c)/kT}\int_{E_c}^{\infty}\left(\frac{E-E_c}{kT}\right)^{\frac{1}{2}} e^{-\frac{(E-E_c)}{kT}}\frac{dE}{kT}$$

LET $X = \frac{E-E_c}{kT}$

$$n = \frac{1}{2\pi^2}\left(\frac{2m_e^*}{\hbar^2}\right)^{3/2}(kT)^{3/2} e^{(E_f-E_c)/kT}\underbrace{\int X^{\frac{1}{2}} e^{-X}\, dX}_{\pi^{1/2}/2}$$

$$\therefore n = \frac{1}{2\pi^2}\left(\frac{2m_e^*}{\hbar^2}\right)^{3/2}(kT)^{3/2} e^{(E_f-E_c)/kT}\ \frac{\pi^{1/2}}{2}$$

$$= 2\left(\frac{2\pi m_e^* kT}{h^2}\right)^{3/2} e^{-(E_c-E_f)/kT}$$

$$= N_c\, e^{-(E_c-E_f)/kT}$$

$p = \int_{\text{BOTTOM OF V BAND}}^{E_V} g(E)[1-f(E)]\,dE$: BOTTOM VALUE $\to -\infty$

$= \frac{1}{2\pi^2}\left(\frac{2m_h^*}{\hbar^2}\right)^{3/2}\int_{-\infty}^{E_V}(E_V-E)^{1/2}\underbrace{\left[1-\frac{1}{e^{(E-E_F)/kT}+1}\right]}_{\substack{\frac{e^{(E-E_F)/kT}}{e^{(E-E_F)/kT}+1} \\ \frac{1}{1+e^{(E_F-E)/kT}}}}dE$

ASSUME $E_f - E \geq 4kT \Rightarrow \frac{1}{1+e^{(E_f-E)/kT}} \simeq e^{(E-E_f)/kT}$

YIELDING

$p = \left(\frac{2\pi m_h^* kT}{h^2}\right)^{3/2} e^{-(E_f-E_V)/kT}$

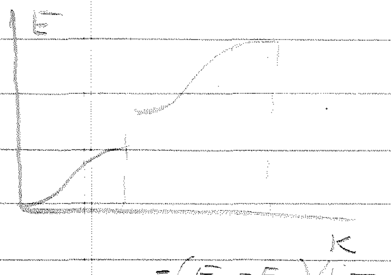
$= N_V\, e^{-(E_f-E_V)/kT}$

INTRINSIC (PURE) SEMICONDUCTOR

SET $n = p$ AND SOLVE FOR E_f

$\Rightarrow E_f = \frac{E_C+E_V}{2} + \frac{3}{4}kT\ln\left(\frac{m_h^*}{m_e^*}\right)$

@ $T = 0°K$, E_F IS HALFWAY 'TWIXT BANDS



$m^* = \frac{\hbar^2}{\delta^2 E/\delta k^2}$

$np = N_C N_V e^{-(E_C-E_V)/kT}$

$= N_C N_V\, e^{-E_g/kT}$

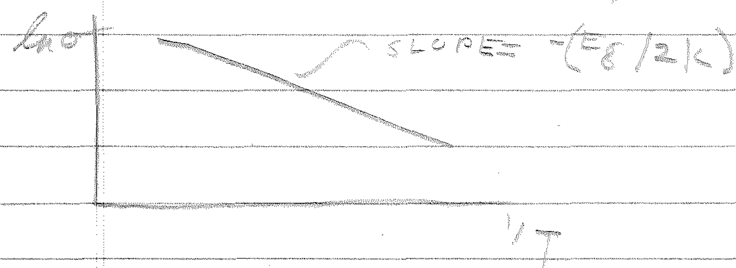
$n = p = \sqrt{np} = (N_C N_V)^{1/2} e^{-E_g/2kT}$

$(N_C N_V)^{1/2} = 2\left(\frac{2\pi kT}{h^2}\right)^{3/2}(m_e^* m_h^*)^{3/4}$

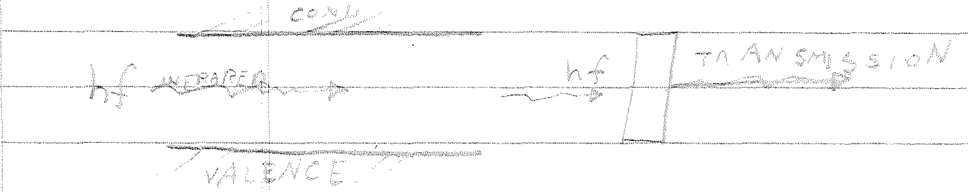
NOW $\sigma = ne\mu_e + pe\mu_h$

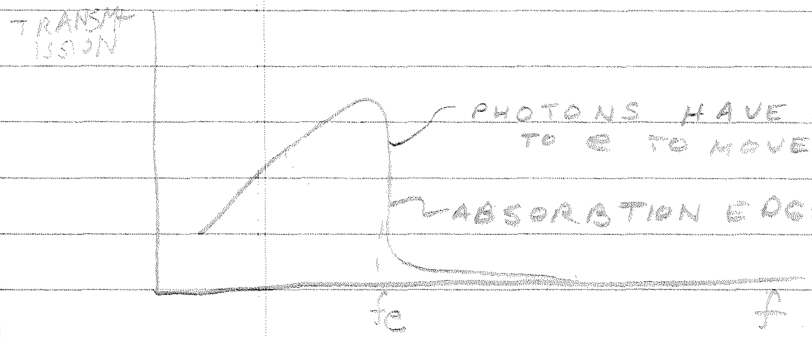
$= \left[(N_C N_V)^{1/2} e^{-E_g/2kT}\right] e(\mu_e + \mu_h)$

$\ln\sigma = \frac{-E_g}{2kT} + \ln\left[(N_C N_V)^{1/2} e(\mu_e+\mu_h)\right]$



DETERMINATION OF E_g BY INFRARED ABSORBSION





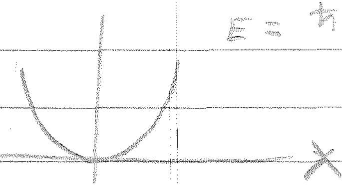
AND $E_g = hf_e$

GO TO Pg 75 (TUES)

5-3-72 (WED)

FREE ELECTRON

$E = \hbar^2 U^2 / 2m$



BOUNDRY CONDITIONS TELL US

1) 2N STATES PER BAND, WHERE N IS NUMBER OF "CELLS" TWIXT ATOMS

VELOCITY OF ELECTRONS IN PERIODIC LATTICE

$V = d\omega / dK$

$E = hf = \hbar\omega \Rightarrow V = \frac{1}{\hbar}\frac{dE}{dK}$

APPLY $\mathcal{E}$ FIELD

$F = q\mathcal{E}$

$dE = F\,dx = F\,v\,dt = \frac{F}{\hbar}\left(\frac{dE}{dK}\right)dt$

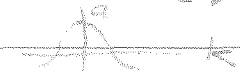
$dE = \frac{dE}{dK}\,dK$

$\frac{F}{\hbar} = \left(\frac{dE}{dK}\right)dt = \frac{dE}{dK}\,dK$

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

$\Rightarrow \frac{dV}{dt} = \frac{1}{\hbar}\,\delta^2 E / \delta h\,\delta t = \frac{1}{\hbar}\frac{\delta^2 E}{\delta K^2}\left(\frac{\delta K}{\delta t}\right) = a$

$= \frac{F}{\hbar^2}\frac{\delta^2 E}{\delta K^2}$



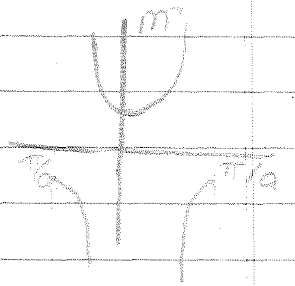
EFFECTIVE MASS

$a = \frac{EF}{m} = \frac{F}{m^*}$

WHEN $\vec{a}$ AND $\vec{F}$ ARE IN OPPOSITE DIRECTOINS, $m^* < 0$

$\frac{F}{\hbar} \frac{\delta^2 E}{\delta k^2} = F/m^*$

$\Rightarrow m^* = \hbar^2 \left(\frac{\delta^2 E}{\delta k^2} \right)^{-1}$



FOR FREE ELECTRONS

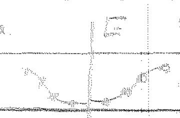
$E = \hbar^2 k^2 / 2m$

$v = \frac{1}{\hbar} \frac{\delta E}{\delta k} = \frac{1}{\hbar} \left(\frac{\hbar^2}{2m} \right) 2k = \frac{\hbar k}{m} = \frac{p}{m}$

$a = F/\hbar^2 \frac{\delta^2 E}{\delta k^2} = \frac{F}{\hbar^2} \frac{\delta}{\delta k} \left(\frac{\hbar^2 k}{m} \right) = \frac{F}{m}$

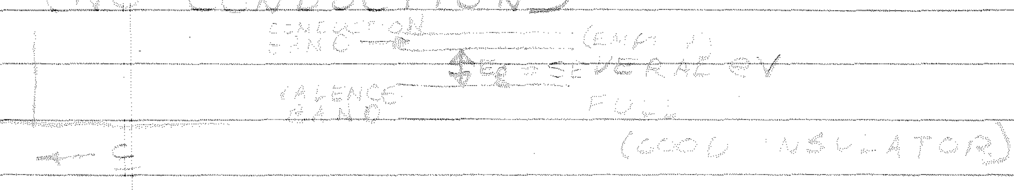
$m^* = \hbar^2 / \ldots m$

CONDUCTION DUE TO FULL BAND = 0

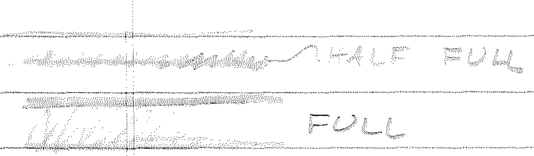


APPLY E TO FULL BAND

YOU CAN'T ACCELERATE THE ELECTRON AS A GROUP (NO CONDUCTION)



METAL



ALKALI-METAL HAVE CONDUCTION BAND HALF FULL

3 DIMENSIONAL CASE

IF OVERLAPPING, OCCURS A METAL

GO TO PG 59 (FRI)

5-16-72 (TUES)

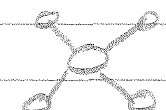
INTRINSIC SEMICONDUCTOR

$$n = p \Rightarrow \begin{cases} E_f = \frac{E_c + E_f}{2} \\ n = p = (N_c N_v)^{\frac{1}{2}} e^{-E_g/kT} \end{cases}$$

FERMI ENERGY IS HALFWAY TWIXT HIGHEST VALENCE E AND LOWEST CONDUCTION E

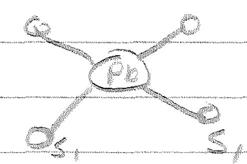
EXTRINSIC (IMPURITY) SEMICONDUCTOR

SILICON

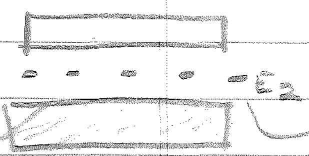


PENTAVALENT IMPURITY

Pb, As



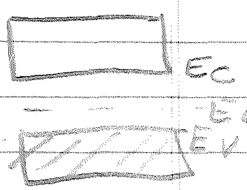
EXTRA-LOOSELY BOUND ELECTRON IN BOHR ORBIT OF BIG RADIUS



DONAR STATES MAY MOVE TO CONDUCTION BAND AT HIGH T AND IONIZING IMPURITY

FOR $n > p$, n TYPE SEMICONDUCTOR

TRI-VALENT IMPURITY WITH S_i ONE EXTRA PLACE FOR e^- IN A BOND



→ ACCEPTOR LEVELS (MT)

AS T↑ A BIT, SOME e^- WILL JUMP TO ACCEPTOR LEVELS, CREATING HOLES IN THE VALENCE BAND.

$p > n \Rightarrow p$ TYPE

N_D = # DONOR LEVELS/VOL

N_D^+ = # IONIZED LEVELS/VOL (LOST e^-'s)

$$n = N_D^+$$

$$N_c e^{-(E_c - E_f)/kT} = N_D\left[1 - f(E)\right]$$

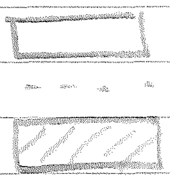
$$= N_D\left[\frac{1}{e^{(E_2 - E_f)/kT} + 1}\right]$$

IF $(E_f - E_2) > 4kT$ (DONOR LEFEL NOT TO CLOSE TO FERMI ENERGY)

$$N_c e^{-(E_c - E_f)/kT} = N_D e^{(E_2 - E_f)/kT}$$

$$\ln N_c + (E_f - E_c)/kT = \ln N_D + (E_2 - E_f)/kT$$

$$\underline{E_f = \frac{E_2 + E_c}{2} + kT \ln(N_D/N_c)}$$



@ $T = 0°K$

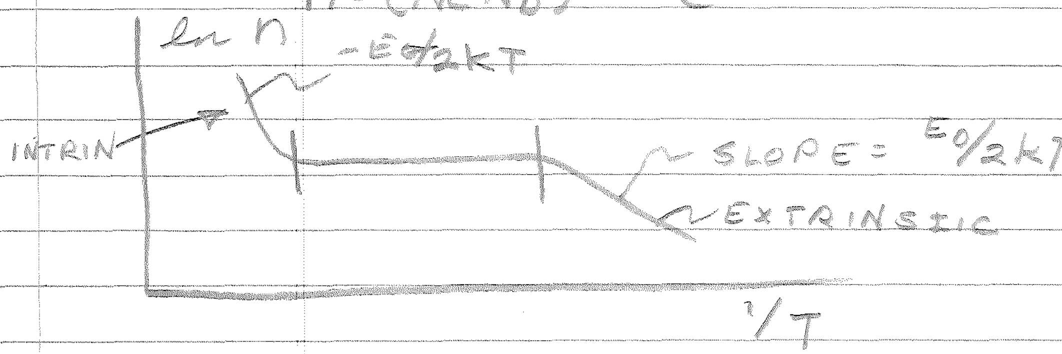
$$n = N_c e^{-(E_c - E_f)/kT}$$

$$\ln n = \ln N_c + \frac{E_f - E_c}{kT}$$

$$= \ln N_c + \frac{1}{kT}\left(\frac{E_c - E_2}{2} + \frac{kT}{2}\ln\left(\frac{N_D}{N_c}\right)\right)$$

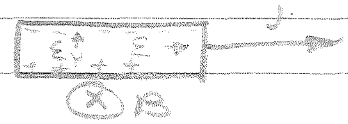
$$= \ln N_c + \frac{1}{2}\ln\left(\frac{N_D}{N_c}\right) - E_D/2kT$$

$$n = (N_c N_D)^{1/2} e^{-E_D/2kT}$$



$\sigma = ne\mu_e$

HALL EFFECT



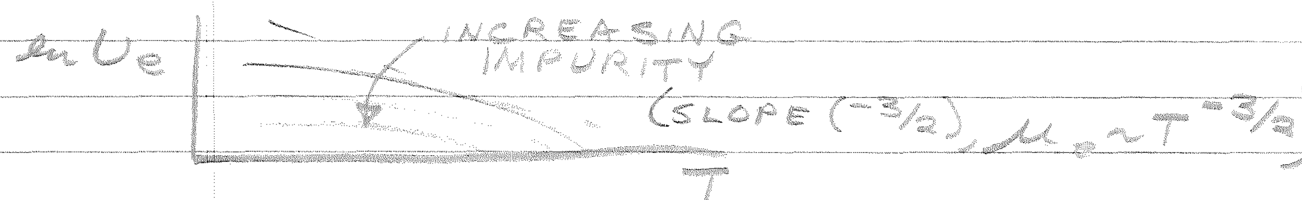
$R_H = \mathcal{E}_y / jB = \frac{1}{ne} \mathcal{E} = V/L$

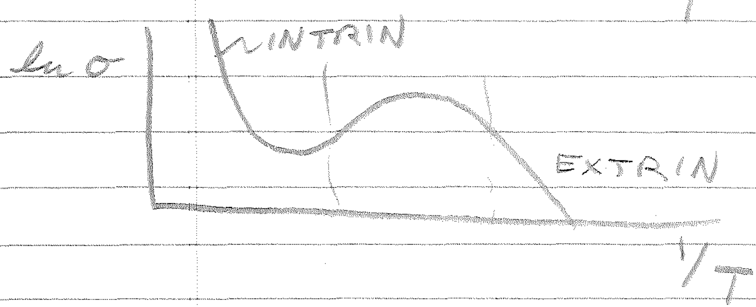
$\sigma = ne^2\tau / m_e^* = ne\mu_e$

$\mu_e = e\tau / m_e^*$

$\mathcal{E}_y = \sigma\mathcal{E}_y / j = \sigma jB / nej = \mu_e B$

MEASURE $\mathcal{E}_y$ & $\mathcal{E}$ & B (HALL MOBILITY)

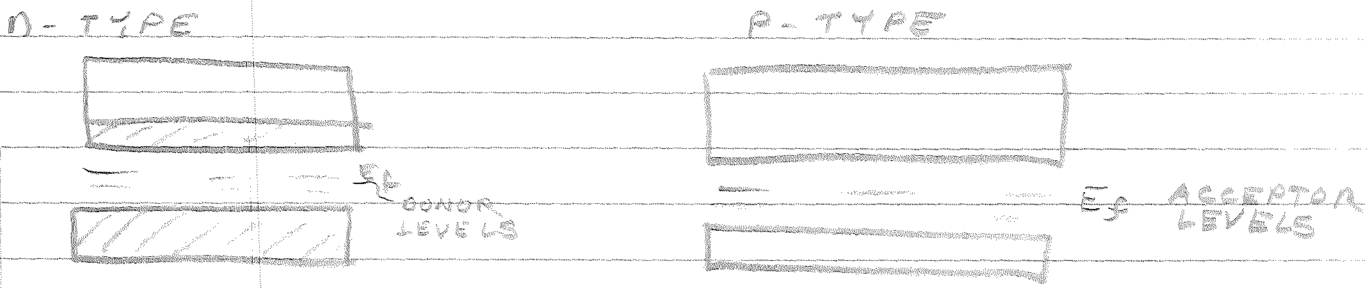




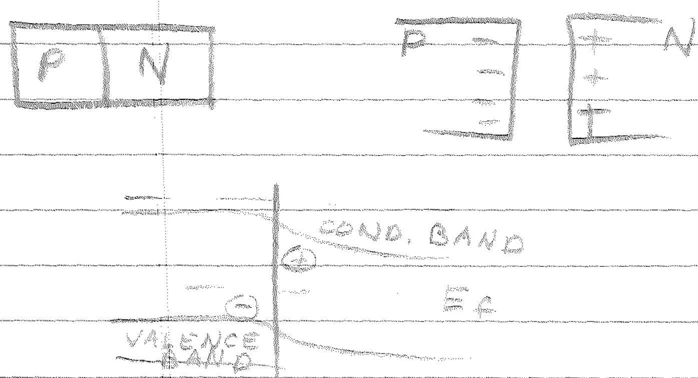
5-17-72 (WED)

n-TYPE

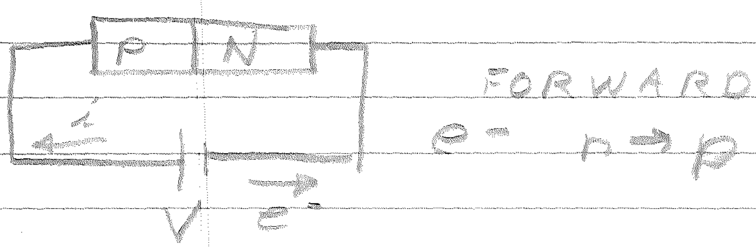
P-TYPE



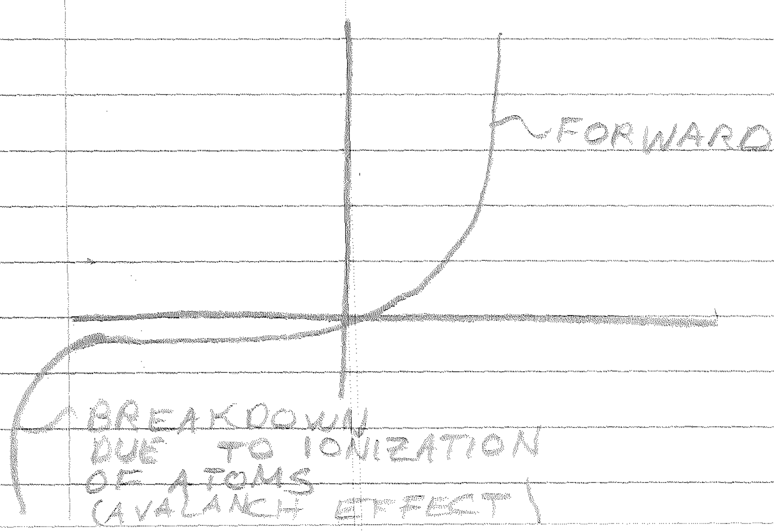
P-N JUNCTION



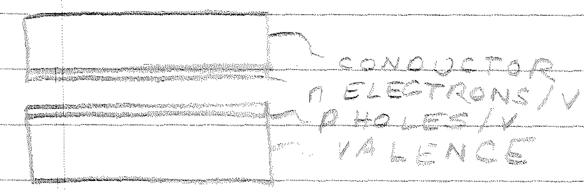
BARRIER FOR DIFFUSION TO LEFT



REVERSE V POLARITY TOO



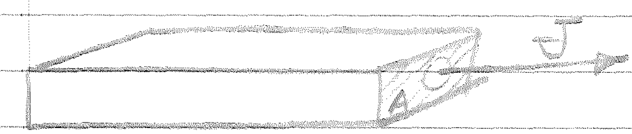
ELECTRON AND HOLE CONDUCTION

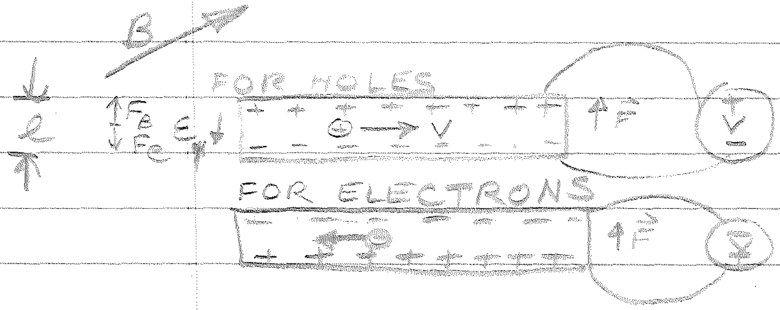


$\sigma = n e \mu_e + p e \mu_h$

$\Rightarrow \mu = $ MOBILITY

HALL EFFECT





$\vec{F} = q\vec{v} \times \vec{B}$

(CAPACITOR ANALOGY)

MAY THUS DETERMINE MAJORITY CARRIERS.

SUPPOSE $p=0,\ n\neq 0$

$$\vec{F} = q\vec{v}\times\vec{B} = qvB = \mathcal{E}_y e = vBe$$

$$\mathcal{E}_y = vB = V/l$$

HALL COEFFICIENT: $R_H \triangleq \mathcal{E}_y / JB$

$$J = I/A$$

$$\Rightarrow R_H = \frac{vB}{JB} = \frac{\cancel{nevB}}{nevB} \quad (nev = J)$$
$$= \frac{1}{ne}$$

THUS MEASURING R_H YIELDS n

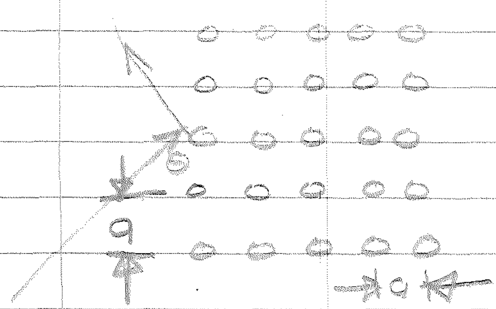
FOR p MATERIAL $R_H = \frac{1}{pe}$

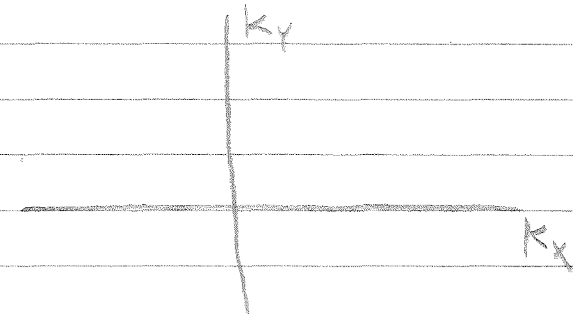
WHEN BOTH TYPES OF CARRIERS ARE IMPORTANT

$$R_H = \frac{1}{e}\left(\frac{p\mu_h^2 - n\mu_e^2}{[p\mu_h + n\mu_e]^2}\right)$$

BANDS IN THREE DIMENSIONS

CUBIC

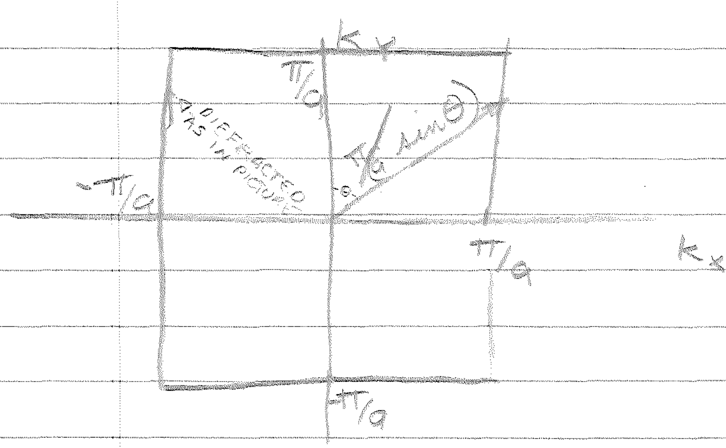




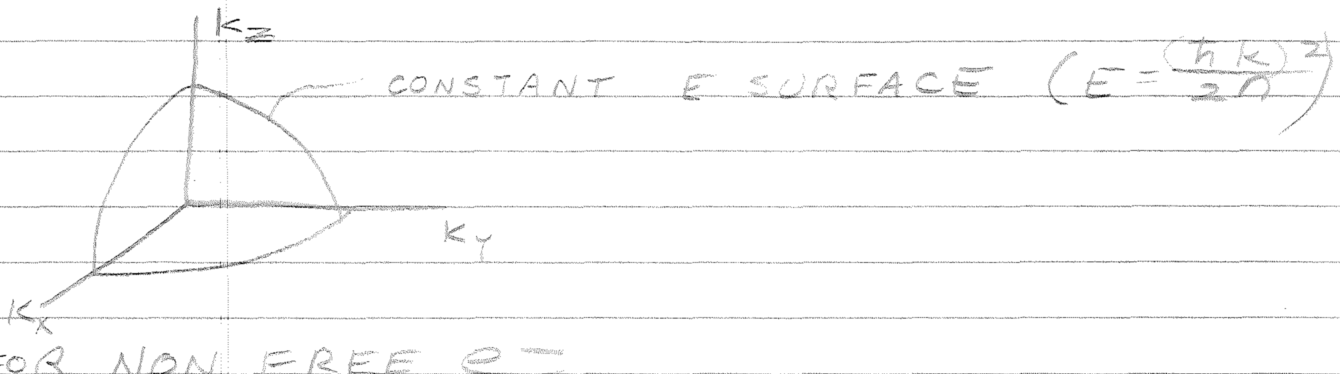
BRAGG'S LAW FOR FIRST ZONE:

$$2a \sin\theta = \lambda$$

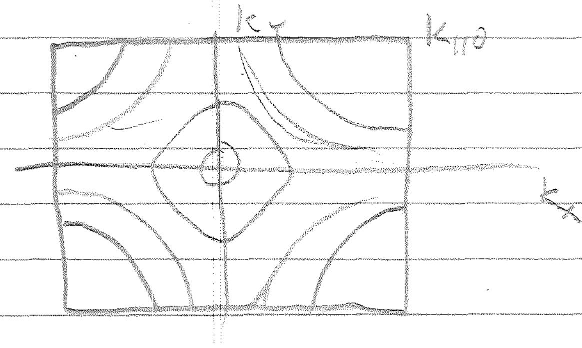
$$\frac{\pi}{a \sin\theta} = \frac{2\pi}{\lambda} = k$$

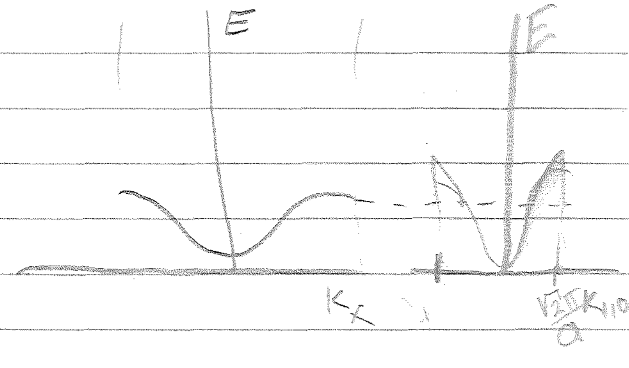


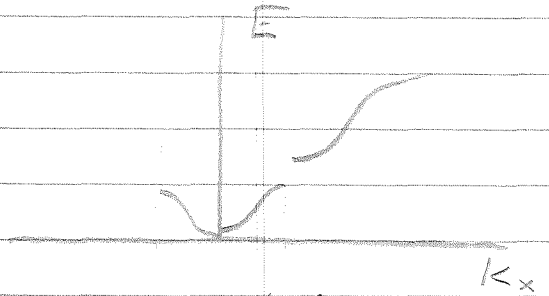
FREE ELECTRON

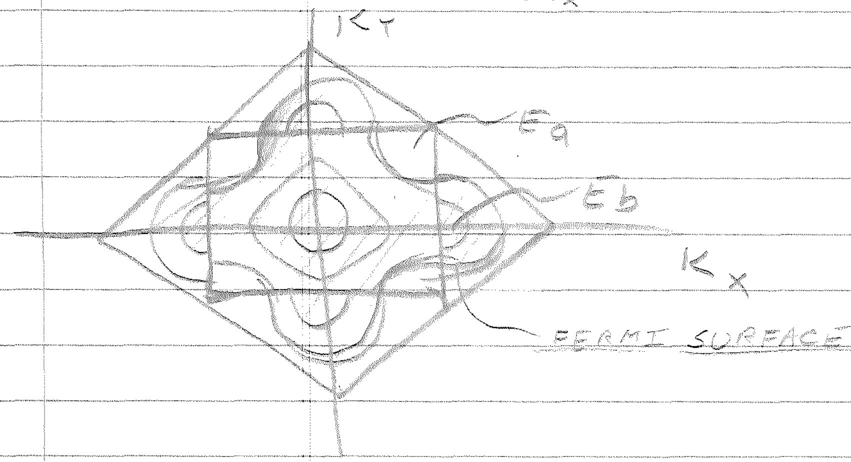


FOR NON FREE e^-







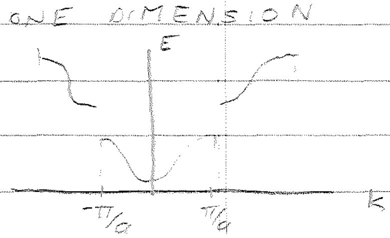


METAL — NO E GAPS $(E_a > E_b)$

SEMICONDUCTOR $E_b < E_a$

5-8-72 (MON)

ONE DIMENSION



$$v = \frac{1}{\hbar}\frac{\delta E}{\delta k}$$

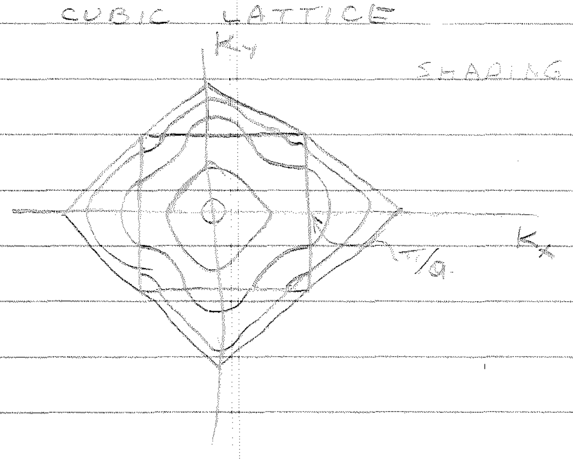
$$\frac{1}{m^*} = \frac{1}{\hbar^2}\frac{\delta^2 E}{\delta k^2}$$

$$\sigma = \frac{ne^2\tau}{m^*}$$

IN THREE DIMENSIONS

CUBIC LATTICE

SHADING → OCCUPIED SPACE



IN 3 DIMENSIONS

$$\vec{V} = \frac{1}{\hbar}\left(\vec{i}\,\frac{\delta E}{\delta k_x} + \vec{j}\,\frac{\delta E}{\delta k_y} + \vec{k}\,\frac{\delta E}{\delta k_z}\right)$$

$$= \frac{1}{\hbar}\nabla_k E$$

$$a_x = \frac{1}{m^*_{xx}}F_x + \frac{1}{m^*_{xy}}F_y + \frac{1}{m^*_{xz}}F_z$$

$$a_y = \frac{1}{m^*_{yx}}F + \frac{1}{m^*_{yy}}F_y + \frac{1}{m^*_{yz}}F_z$$

$$a_z = \frac{1}{m^*_{zx}} + \frac{1}{m^*_{zy}} + \frac{1}{m^*_{zz}}F_z$$

$$\frac{1}{m^*_{ij}} = \frac{1}{\hbar^2}\frac{\delta^2 E}{\delta k_i \delta k_j}$$

FREE ELECTRONS

$$E = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2}{2m}\left(k_x^2 + k_y^2 + k_z^2\right)$$

$$\vec{V} = \frac{1}{\hbar}\left(\vec{i}\,\frac{\hbar^2 k_x}{m} + \vec{j}\,\frac{\hbar^2 k_y}{m} + \frac{\hbar^2 k_z}{m}\vec{k}\right)$$

$$= \frac{\hbar}{m}\left(k_x\vec{i} + k_y\vec{j} + k_z\vec{k}\right)$$

$$= \frac{\hbar\vec{k}}{m} = \vec{P}/m$$

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

$$= \hbar^2\left(k_x^2 + k_y^2 + k_z^2\right)/2m$$

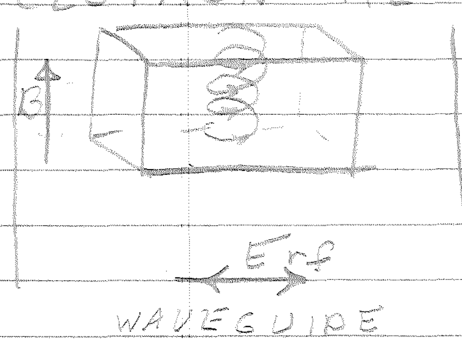
$$\left(\frac{1}{m^*_{xx}}\right) = \frac{1}{\hbar^2}\frac{\hbar^2}{m} = \frac{1}{m}$$

$$\left(\frac{1}{m^*_{yy}}\right) = \left(\frac{1}{m^*_{zz}}\right) = \frac{1}{m};$$ ALL OTHERS = 0

THEN:

$$a_x = \frac{1}{m}F_x;\ a_y = \frac{1}{m}F_y;\ a_z = \frac{1}{m}F_z$$

CYCLOTRON RESONANCE FREQ.



$B \perp E_{rf}$

ELECTRON MOVING UPWARD Q < WITH ENERGY NEAR E_f (FERMI ENERGY)

$$F_{CENTRIC} = Bqv = m^*\omega^2 r$$

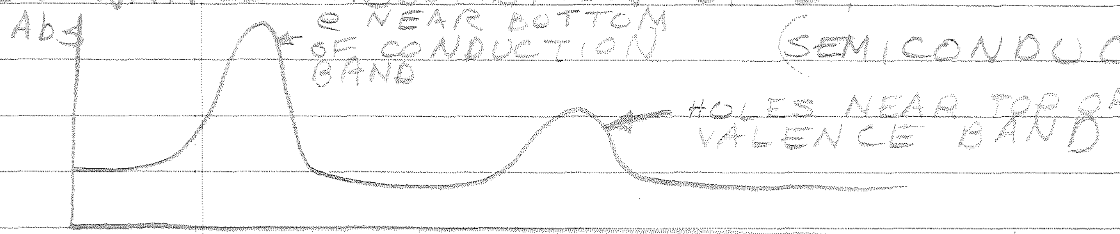
$$\omega_c = Bq/m^*$$

IF RADIO FREQUENCY MATCHES ω_c, THEN ONE COULD GET A LARGE AMOUNT OF ABSORBTION OF ENERGY FROM rf.

(CHANGE B AND LOOK FOR ABSORPTION RESONANCE

CHANGE B AND LOOK FOR LARGE RESONANCE ABSORBTION OF E

(SEMICONDUCTOR)



B IN SOME PARTICULAR DIRECTION

$k = \frac{2\pi n}{Na}$ $n = \pm 1, \pm 2, \ldots$ (ONE DIMENSION)

STATES IN FIRST BAND

IN THREE DIMENSIONS

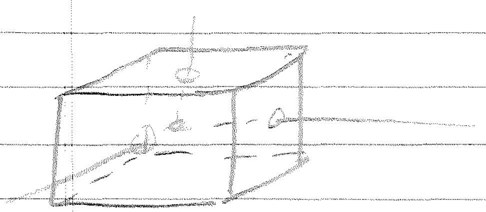
$\longleftarrow L = Na \longrightarrow$

$\psi(x)$ $\qquad$ $\psi(x+L)$

$k_x = \frac{2\pi n_x}{Na}$ $\qquad n_x = \pm 1, \pm 2, \ldots$

$k_y = \frac{2\pi n_y}{Na}$ $\qquad n_y =$ 〃

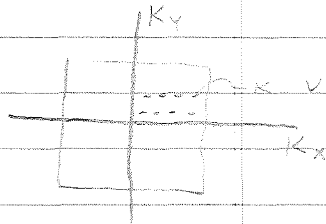
$k_z = 2\pi n_z / Na$ $\qquad n_z =$ 〃



NUMBER OF STATES (w 2 STATES/POINT (e-SPIN))

N^3 = NO. OF UNITCELLS IN LATTICE

5-9-72 (TUES)

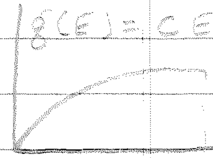


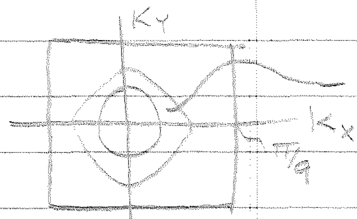
K VECTORS MAY END ON THESE POINTS

CYCLIC BOUNDRY CONDITION: $\psi(x) = \psi(x+L)$

NEED TO KNOW HOW ENERGY IS DISTRIBUTED TO KNOW CONDUCTION

$g(E) = CE^{\frac{1}{2}}$ FOR FREE e^-





HOW MANY STATES TWIXT E & dE $(g(E)dE)$

VOLUME OF FIRST ZONE IN K SPACE

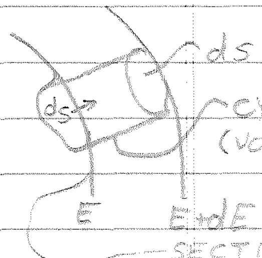
$$\Omega = \left(\frac{2\pi}{a}\right)^3$$

DENSITY OF STATES IN K SPACE

$$\frac{dn}{d\Omega} = \frac{2N^3}{8\pi^3/a^3} = \frac{2N^3a^3}{8\pi^3} \ni (Na)^3 = \text{VOLUME OF CRYSTAL}$$

$$\Rightarrow \frac{dn}{d\Omega} = \frac{2}{8\pi^3} \text{ STATES/UNIT VOLUME IN K SPACE}$$

$g(E)dE = \frac{dn}{d\Omega} \times$ VOLUME TWIXT ENERGY SURFACE E & E+dE (IN K SPACE)



ds = SURFACE ELEMENT

CYLINDER (VOLUME = $dK_n ds$)

SECTION OF ENERGY SURFACE

dK_n IS THE CHANGE IN K GOING FROM E TO E+dE IN THE NORMAL DIRECTION

$$dE = |\nabla_K E|\, dK_n = |\text{GRAD}_K E|\, dK_n \Rightarrow dK_n = \frac{dE}{|\Delta_K E|}$$

THUS $g(E)dE = \frac{2}{8\pi^3} dK_n \int dS$ (INTEGRATE OVER CONST. EN. SURFACE)

$dK_n \int dS$ = TOTAL VOLUME TWIXT E AND E+dE

EXAMPLE - FREE ELECTRON

$$E = \frac{\hbar^2}{2m}(k_x^2 + k_y^2 + k_z^2)$$

$$\nabla E = \vec{i}\frac{\partial E}{\partial x} + \vec{j}\frac{\partial E}{\partial y} + \vec{k}\frac{\partial E}{\partial z}$$

$$= \frac{\hbar^2}{2m}(2k_x\vec{i} + 2k_y\vec{j} + 2k_z\vec{k})$$

$$= \frac{\hbar^2}{m}\vec{k} \Rightarrow |\nabla_k E| = \frac{\hbar^2 k}{m}$$ ∋ k IS NOT A VECTOR

THIS IS EXPRESSION FOR CONSTANT E SURFACE

$\Rightarrow \int ds = 4\pi k^2$ ∋ $\int$ IS OVER CONSTANT E SURFACE

$$\Rightarrow g(E)\,dE = \frac{2}{8\pi^3}\frac{dE}{\hbar^2 k/m}(4\pi k^2)$$

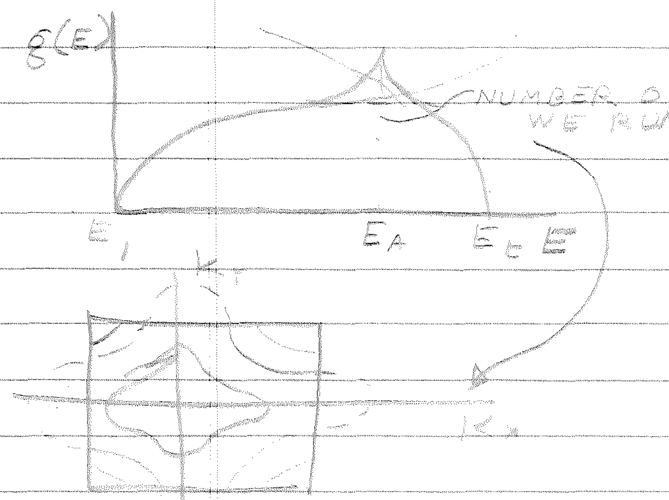
$$\therefore g(E) = \frac{mk}{\pi^2\hbar^2} = \frac{1}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} E^{1/2} = C E^{1/2}$$

BECAUSE $k = \sqrt{\frac{2mE}{\hbar^2}}$ FROM $E = \hbar^2 k^2/2m$

THE PREVIOUSLY DERIVED ANSWER

SOME OTHER RESULTS

ELECTRON IN A CRYSTAL (GENERALLY NOT FREE)



NEAR THE BOTTOM OF THE BAND:

$$g(E) = \frac{1}{2\pi^2}\left(\frac{2m^*}{\hbar^2}\right)^{3/2}(E - E_B)^{1/2}$$

ASSUMING WE'RE NOT IN THE FIRST BAND. $E_B = 0$ IN FIRST BAND

NEAR THE TOP OF THE BAND

$$g(E) = \frac{1}{2\pi^2}\left(\frac{2m^*}{\hbar^2}\right)^{3/2}(E_T - E)^{1/2}$$

ELECTRONS NEAR THE TOP AND BOTTOM OF THE BANDS ARE THE ONES GENERALLY THE ONLY ONES OF INTEREST

ALKALI METALS HAVE TWICE AS MANY STATES AS THEY HAVE ELECTRONS TO PUT IN THEM, YIELDING HALF FULL BANDS. THIS GUARATEES IT IS A METAL

GOOD CONDUCTOR ⇒ CHANGES STATE EASILY

CALCIUM (DIVALENT METALS): 2 VALENE ELECTRONS - AS MANY ELECTRONS AS STATES, SINCE IT IS METAL, MUST HAVE BAND OVERLAP

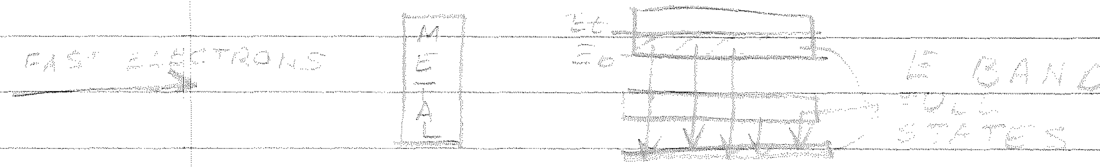
TRANSITION METALS - OVERLAPING BAND, LARGE m^*; NOT A GOOD CONDUCTOR. (NARROW BAND / WIDE BAND)

$m^* = \hbar^2 \left(\frac{\delta^2 E}{\delta k^2} \right)^{-1}$; IF BAND IS NARROW, m^* IS LARGE ⇒ NARROW BAND IS POOR CONDUCTOR SINCE m^* IS HARD TO ACCELERATE

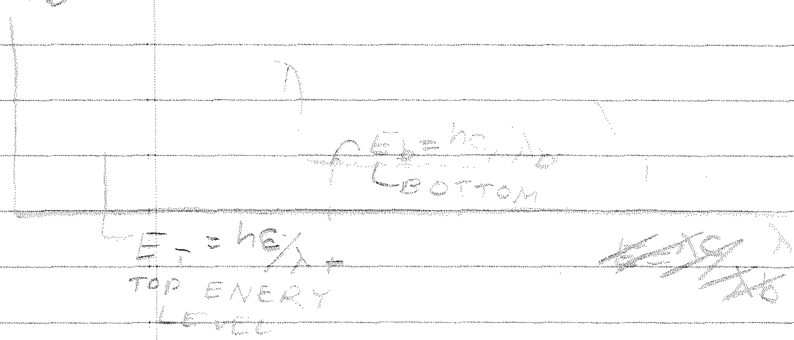
DIAMOND - GAP OF ENERGY: $E_g = 7 eV$ (BIG) HARD TO BRIDGE GAP. FULL AND EMPTY BAND SEPARATED BY E_g

GERMANIUM - SIMILAR TO DIAMOND, BUT $E_g = .7 eV$, SO SOME ELECTRONS CAN JUMP GAP AFTER ABSORBING PHONON (IF $T > 0°K$) AND ENTER THE CONDUCTION BAND. NUMBER OF ELECTRON BAND LIMITED (UNLIKE METALS) ⇒ SEMICONDUCTOR

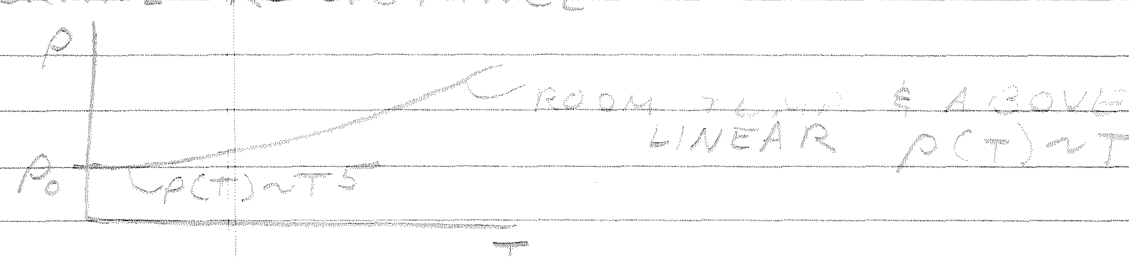
HOW TO INVESTIGATE BANDS (EXPERIMENT)



KNOCK OUT ELECTRON FROM LOWER LEVEL, SO [illegible] ELECTRON DROPS AND EMITS X-RAYS



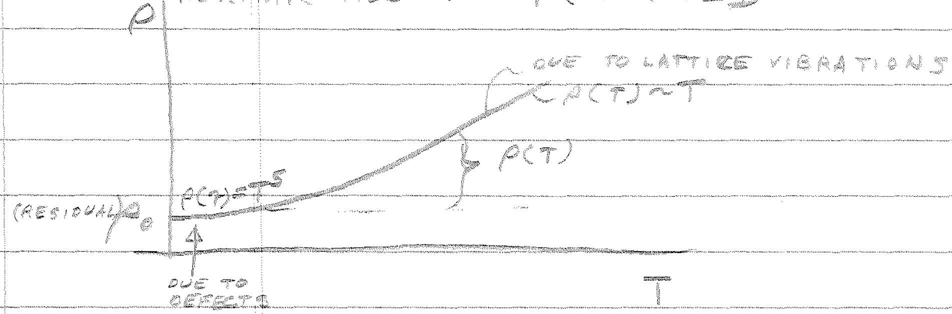
NORMAL RESISTANCE



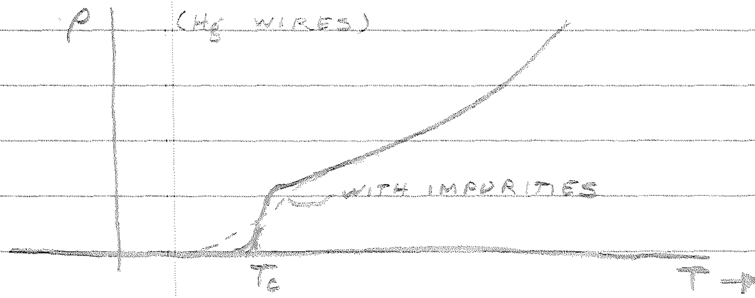
ρ_0 IS RESIDUAL RESISTANCE, DUE TO LATTICE DEFECTS & IMPURITIES
ρ @ ROOM TEMPERATURE & ABOVE IS DEPENDENT ON LATTICE VIBRATIONS
∴ FOR SUPER-CONDUCTIVITY, WE MUST ∴ DO AWAY WITH THE PROBLEM OF DEFECTS AND IMPURITIES

5-10-71 (WED)

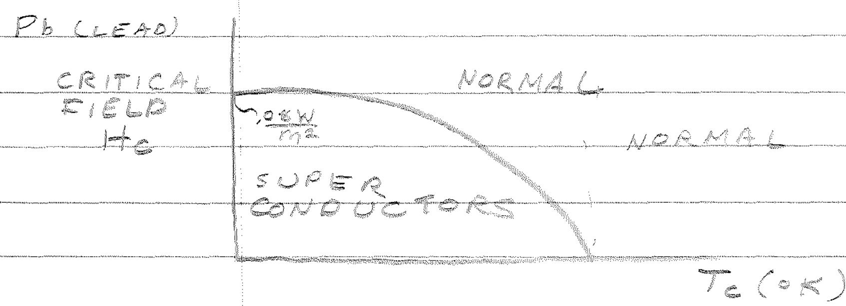
NORMAR RESISTIVITY (METALS)



ONNES - 1911 - SUPERCONDUCTIVITY



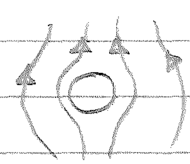
∃ 23 SUPERCONDUCTOR ELEMENTS, & HUNDREDS OF ALLOYS



BEST SUPERCONDUCTORS ARE POOREST NORMAL CONDUCTORS

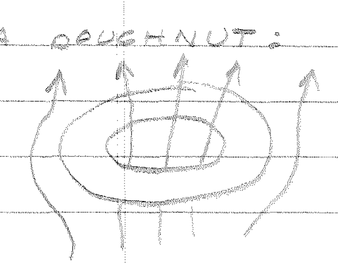
APPLY MAGNETIC FIELD AND TAKE DOWNWARD THRU T_c → SURFACE CURRENT SET UP THAT CANCELS FIELD INSIDE THE SUPER-CONDUCTOR (MEISSNER EFFECT)

$T < T_c$

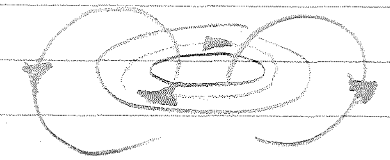


FOR A DOUGHNUT:

FIELD ON



FIELD OFF TRAPS LINES
GIVING MAGNET WITH CURRENT



ISOTOPE EFFECT

$T_c \sim \frac{1}{\sqrt{M}}$ $\ni$ M = MASS OF THE ATOM (FOR PARTICULAR ATOM)

$\Rightarrow$ LESS INERTIA $\Rightarrow$ LESS MOVEABLE

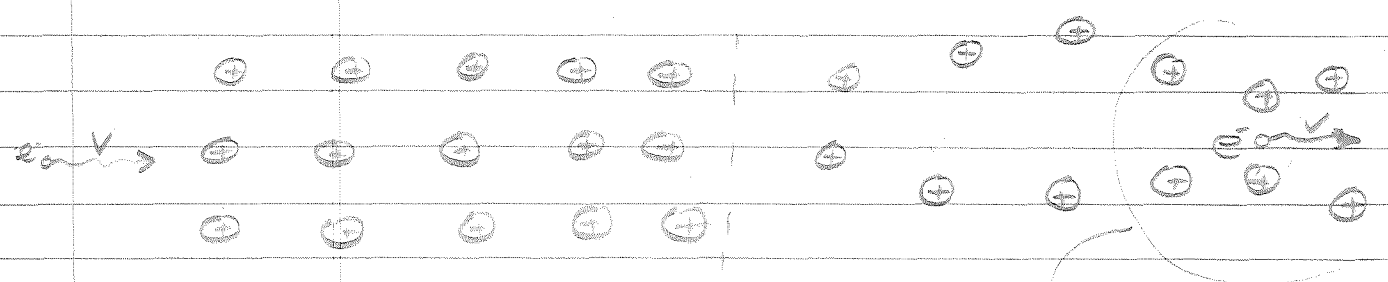
$\Rightarrow$ HIGHER T_c $\Rightarrow$ BETTER SUPERCONDUCTIVITY

(EFFECT CAUSING SUPER-CONDUCTIVITY IS STRONGER)

THEORY DEVELOPED IN 1958

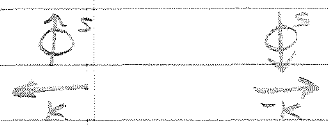
BCS THEORY (BARDEEN, COOPER, SCHRIEFFER)

SIMPLIFIED BCS THEORY



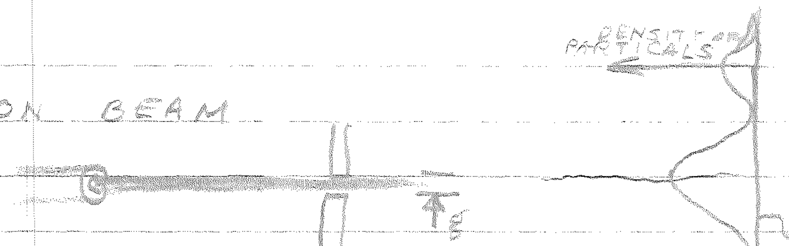
HI + DENSITY

ANOTHER e^- MIGHT BE ATTRACTED TO REGION OF HIGH DENSITY CHARGE.
PAIRS OF ATTRACTING ELECTRONS (VIA LATTICE WAVES). ELECTRONS HAVING LOWER ENERGIES THAN SINGLE ELECTRONS WOULD HAVE



COOPER PAIRS WILL REACT UP TO 10^{-4} CM

ELECTRON BEAM



MAY DETERMINE λ FROM ABOVE

CAN ALSO DETERMINE P (MOMENTUM)

AGAIN: $P = h/\lambda$; $E = P^2/2m + V$ POTENTIAL ENERGY

DUAL NATURE OF WAVE-PARICLES

(1) LIGHT ; $E = hf$ $\quad p = \hbar k \quad k = \frac{2\pi}{\lambda}$

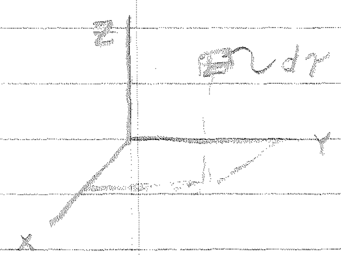
2) MATTER, $p = \hbar k \quad E = p^2/2m$

HEISENBURG UNCERTAINTY PRINCIPLE:

IT IS IMPOSSIBLE TO SIMULTANEOUSLY DETERMINE A POSITITION COORDINATE AND THE CORRESPONDING MOMENTUM COORDINATE TO ANY GREATER PRECISION THAN: $(\Delta p_x)(\Delta x) \geq h$

INVENT "WAVE FUNCTION" : ψ (HAS VALUE AT ALL POINTS IN SPACE, CAN BE REAL OR COMPLEX)

THE PROBABILITY OF FINDING A PARTICAL IN VOLUME ELEMENT $d\tau$ AT POSITION x, y, z IS = PROB = $|\psi(x,y,z)|^2 d\tau$



PROBABILITY OF BEING IN SOME FINITE VOLUME τ:

$$P = \int_\tau |\psi|^2 d\tau$$

SCHROEDINGER EQUATION (CONSERVATION OF E FOR WAVE)

FOR TIME INDEPENDANCE: ie) $|\Psi|^2$ IS NOT FUNCTION OF T

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = E\psi$$

EX) VIBRATING ATOM (LINEAR HARMONIC OSCILLATOR):

$$V = \frac{1}{2}kx^2$$

$$\Rightarrow \frac{-\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + \frac{1}{2}kx^2\psi = E\psi$$

UPON SOLUTION, A SET OF Ψ'S IS OBTAINED. FOR EACH Ψ THE IS A DISCRETE ENERGY (E) IN ORDER TO SATISFY DIFFERENTIAL EQUATION

STATE 1: Ψ_1 —— E_1

" 2: Ψ_2 —— E_2

ETC.

∴ ENERGY IS QUANTIZED

$$\left(E_n = \frac{(2n-1)}{2}hf\right) \quad n=1,2,3$$

[NO SOLUTION FOR E=0: ERGO ATOM IS NEVER AT REST]

3-15-72 (WED)

LEVY: pp. 3-22

NOTES

(1) WAVE PARTICLE DUALITY

(a) LIGHT $E = hf$ $p = \hbar$ $k = 2\pi/\lambda$

(b) MATTER $E = mc^2 = \frac{p^2}{2m}$ $p = \hbar k$

(2) UNCERTAINTY → $P = \int_\tau |\Psi|^2 d\tau$

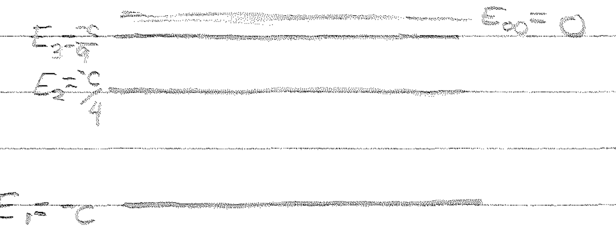
$$\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = E\psi \quad \text{(SCROEDINGER'S EQU. TIME INDEP.)}$$

(3) ONE ELECTRON ATOM: $V = \frac{1}{4\pi\epsilon_0}\frac{q^2}{r}$

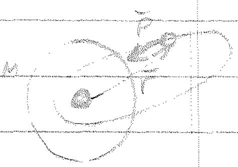
YIELDING THE FOLLOWING RESULTS:

$$E = \frac{-C}{n^2} \ni n = 1, 2, 3, \ldots$$

= PRINCIPLE QUANTUM NUMBER



ATOM



$\ell = \vec{r} \times \vec{p}$ (ANGULAR MOMENTUM)

BOTH HAVE SAME $\bar{E}$, BUT HAVE DIFFERENT $\bar{\ell}$

ALLOWED ANGULAR MOMENTA (ORBITAL)

$$|\vec{\ell}| = \sqrt{\ell(\ell+1)}\,\hbar \;;\; \ell = n-1, n-2, n-3, \ldots, 0$$

ℓ CALLED AZIMUTHAL QUANTUM NUMBER

SUPPOSE $n = 2$, THEN $\ell = 1, 0$

$\Rightarrow |\vec{\ell}| = \sqrt{2}\,\hbar$ OR $|\vec{\ell}| = 0$

$\ell = 0 \Rightarrow s$ ELECTRON

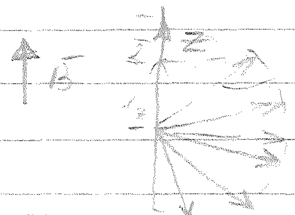
$\ell = 1 \Rightarrow p$ ELECTRON

$\ell = 2 \Rightarrow d$ ELECTRON

$\ell = 3 \Rightarrow f$ ELECTRON

ELECTRON SPIN ANGULAR MOMENTUM $\left(|\vec{S}| = \sqrt{s(s+1)}\,\hbar \Rightarrow s = \tfrac{1}{2}\right.$
$\left. = \sqrt{3/4}\,\hbar\right)$

IN PRESENCE OF MAGNETIC FIELD, ONLY CERTAIN DIRECTIONS ALLOWED FOR $\bar{\ell}$ AND $\bar{s}$ VECTOR:

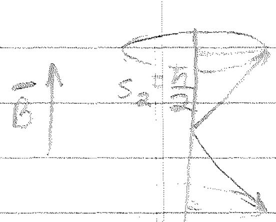


$\ell_z = m\hbar \Rightarrow m = 2, 1, 0, -1, -2$

$\Rightarrow \ell_z = 2\hbar, \hbar, 0, -\hbar, -2\hbar$

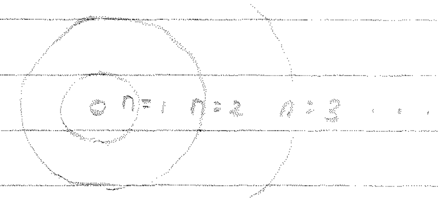
LET $\ell = 2 \Rightarrow |\vec{\ell}| = \sqrt{6}\,\hbar$

$S_z = m_s \hbar \Rightarrow m_s = \pm \frac{1}{2}$



PAULI-EXCLUSION PRINCIPLE (APPLIES TO ODD HALF INTEGRAL SPIN PARTICLES): NO TWO EXECTRONS (ODD HALF INTEGRAL SPIN PARTICLES IN THE SAME (QUANTUM MECHANICAL SYSTEM) ATOM MAY HAVE IDENTICAL SETS OF QUANTUM NUMBERS (n, ℓ, m, m_s)

$$\begin{array}{lccccl} & n & \ell & m & m_s & \\ H: & (1 & 0 & 0 & +\tfrac{1}{2}) & 1s \\ He: & 1 & 0 & 0 & +\tfrac{1}{2} & 1s^2 \\ & 1 & 0 & 0 & -\tfrac{1}{2} & \\ Li: & 1 & 0 & 0 & +\tfrac{1}{2} & 1s^2 2s \\ & 1 & 0 & 0 & -\tfrac{1}{2} & \\ & 2 & 0 & 0 & +\tfrac{1}{2} & \end{array}$$



Be $1s^2 2s^2$

B $1s^2 2s^2 2p$ $\quad 2p: (2, 1, 0, +\tfrac{1}{2})$

C $\quad 2p^2: (2, 1, 0, +\tfrac{1}{2})$

N $\quad 2p^3: (2, 1, -1, +\tfrac{1}{2})$

O $\quad 2p^4: (2, 1, 1, -\tfrac{1}{2})$

F $\quad 2p^5: (2, 1, -1, -\tfrac{1}{2})$

Ne $\quad 2p^6: (2, 1, 1, -\tfrac{1}{2})$

n: ENERGY

ℓ: ORBITAL ANGULAR MOMENTUM

m: Z DIRECTIONAL COMPONENT OF $\vec{\ell}$

m_s: Z COMPONENT OF $\vec{s}$

$s = \pm\frac{1}{2}$

CRYSTALLINE SOLIDS ← REGULAR ATOM ARRANGEMENTS

AMORPHONE SOLIDS ← RANDOM (BUMMERS TO ANALIZE)

FORCES TWIXT ATOMS

A) IONIC FORCES (Na^+ Cl^-)

— COULOMB ATTRACTION OF IONS

— STRONG FORCE

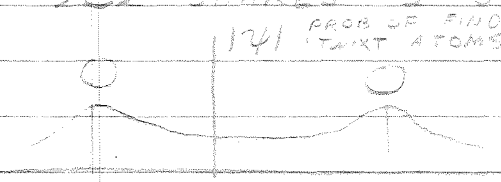
HIGH MELTING POINT

LOW ELECTRICAL-THERMAL CONDUCTION

B) COVALENT FORCE (SHARED ELECTRONS)

$2Cl$ SHARES 2 3P ELECTRONS

$|\psi|$ PROB OF FIND NO e TWIXT ATOMS

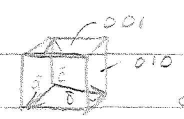


EXCESS NEGATIVE CHARGE

FAIRLY STRONG FORCE

(GO TO FRIDAY, Pg 9)

3-20-72 MON) TEST NEXT WEEK (DO Pg 4-55)

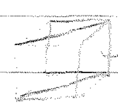


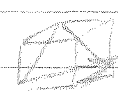
$a = b = c$

$\alpha = \beta = \gamma = 90°$

FRONT FACE

$(1, \infty, \infty)$ TAKE RECIPROCALS: $(1, 0, 0) = hkl$ (MILLER INDICIES


(0, 1, 0)


(1 1 1)

$\{100\} = (100), (010), (001)$

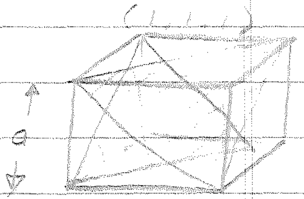
DESIGNATION OF POINTS IN UNIT CELL

BODY CENTERED POSITION IS $(\frac{1}{2}\ \frac{1}{2}\ \frac{1}{2})$

FOR BODY CENTRAL POSITION

POSITION $(\frac{1}{2}\ \frac{1}{2}, \frac{1}{4}) \Rightarrow (1, 1, \frac{3}{4})$

SPACING 'TWIXT PLAINS CONTAINING LATTICE POINTS (PRIMITIVE CELL)



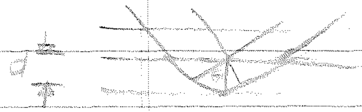
$\{100\} \quad d = a$

$\{110\} \quad d = \frac{a}{\sqrt{2}}$

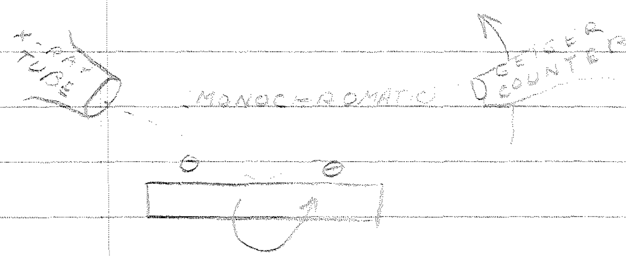
$(111) \quad d = \frac{a}{\sqrt{3}}$

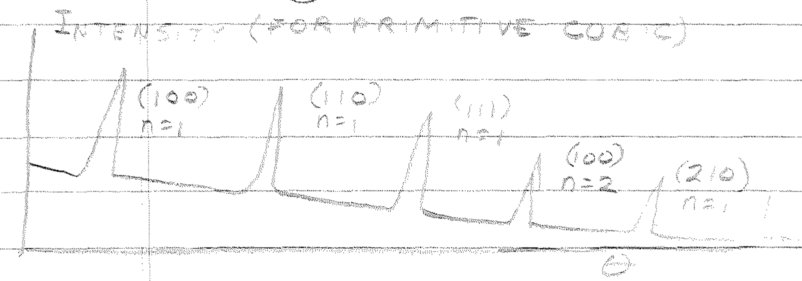
$$d = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

X-RAY DIFFRACTION DETERMINATION OF UNIT CELLS



IF $2d \sin\theta = n\lambda$: CONSTRUCTIVE INTERFERENCE (BRAGG'S LAW)





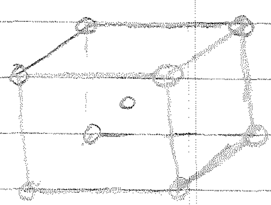
PRIMITIVE CUBIC: $d = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$

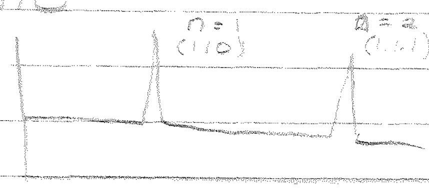
$$2d \sin\theta = n\lambda$$

$$\Rightarrow \sin\theta = \frac{n\lambda\sqrt{h^2 + k^2 + l^2}}{2a}$$

SOLVE FOR a (LATTICE CONSTANT)

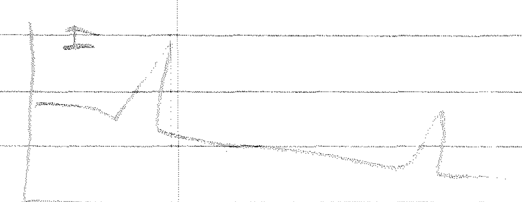
BODY CENTERED CUBIC





(KNOCKS OUT EVERY OTHER PEAK)

n(hkl)	CUBIC PRIMITIVE	CUBIC BODY CENTER	CUBIC FACE CENTER
100	✓	—	✓
110	✓	✓	—
111	✓	—	—
200	✓	✓	✓
210	✓	—	✓
211	✓	✓	—
220	✓	✓	—
221	✓	—	✓



GIVEN A 2θ POSITION OF PEAKS

(1) ASSUME FIRST PEAK IS (100) → CALCULATE a
- SEE IF OTHER PEAKS FIT WITH THIS VALUE OF a AND SOME hkl

(2) ASSUME BCC, FIRST PEAK $(hkl) = 110$
CALCULATE a - SEE IF OTHER PEAKS FIT

(3) ASSUME FCC, FIRST PEAK $(hkl) = (111)$
CALCULATE a - SEE IF OTHER PEAKS FIT

3-17-72 (FRI)

FORCES 'TWIXT ATOMS

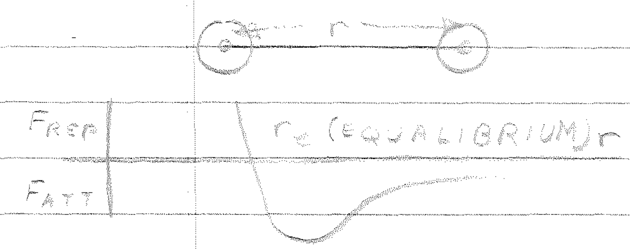
1) IONIC (STRONG ATTRACTION)

2) COVALENT (FAIRLY STRONG)

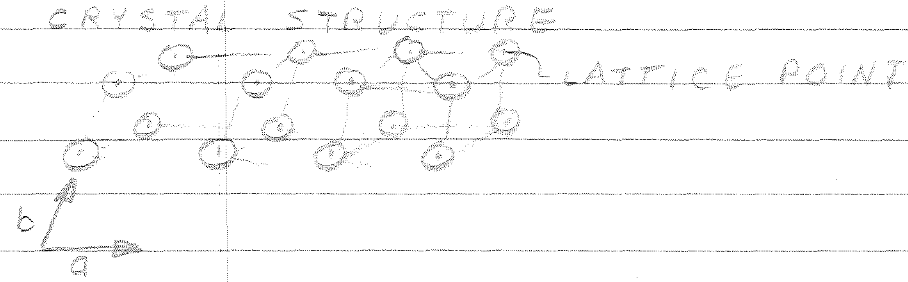
3) METALLIC BOND (SHARED ELECTRONS 'TWIXT ALL ATOMS OF THE MATERIAL

4) VAN-DER WAALS FORCE (MOLECULAR CRYSTALS)
VERY WEAK DIPOLE ATTRACTIVE FORCE
THESE MATERIALS ARE SOLIDS ONLY AT TEMPS NEAR 0° K

5) REPULSIVE FORCES (DUE TO EXCLUSION PRINCIPLE)



CRYSTAL STRUCTURE



SPACE LATTICE: REGULAR (REPEATING) ARRANGEMENT OF POINTS SUCH THAT THE ARRANGEMENT OF ATOMS ABOUT EACH POINT IS IDENTICAL

TO GET FROM ONE LATTICE POINT TO ANY OTHER LATTICE POINT

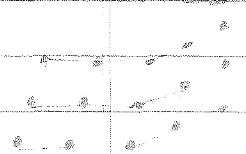
$\vec{T} = m_1\vec{a} + m_2\vec{b} + m_3\vec{c}$

THE VOLUME FOR WHICH $\vec{a}$, $\vec{b}$ AND $\vec{c}$ INSCRIBE THE EDGES IS CALLED A "UNIT CELL"

PRIMITIVE UNIT CELL - THAT CELL HAVING SMALLEST POSSIBLE VOLUME (LATTICE POINTS ONLY @ CORNERS)

SINGLE CRYSTAL = LATTICE CONTINUES FROM ONE EDGE OF CRYSTAL TO THE OTHER WITH NO BREAKS

POLYCRYSTALLINE - BREAKS IN THE LATTICE



GRAIN BOUNDRY

SPACE LATTICE SYMMETRY

(1) MIRROR PLANE

(2) ROTATION SYMMETRY (n-FOLD)

n = THE NUMBER OF EQUAL ANGLES OF ROTATION TO GET BACK TO ORIGINAL CONFIGURATION (EACH OF THE EQUAL ROTATIONS MUST YIELD THE SAME CONFIGURATION AS ORIGINAL)

CUBIC CRYSTALS: 4-3 FOLD ROTATION AXES

MILLER INDICES

(1) INTERCEPTS

(2) RECIPROCAL

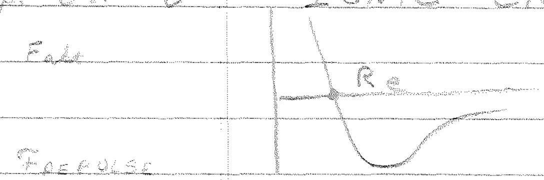
(3) CLEAR FRACTIONS

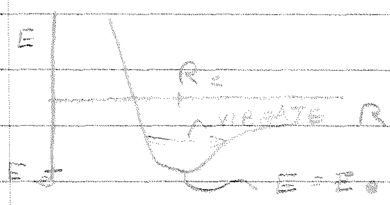
GO TO MONDAY Pg 6

~~GO TO TUESDAY! pg 15~~

3-22-71 WED

pp. 82-98 IONIC CRYSTALS

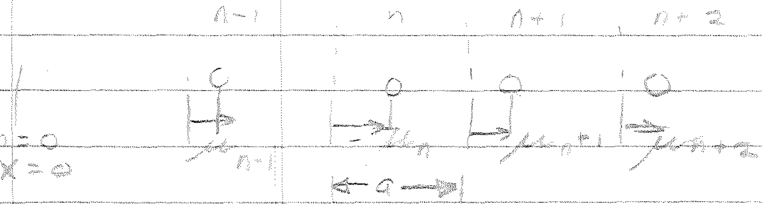




$E = E_0 + \frac{1}{2}Bx^2$ (x DISTANCE FROM R_e)

RESTORING FORCE: $F = Bx$

VIBRATIONS



CONSIDER FORCES BETWEEN ADJACENT ATOMS

$$\vec{F}_n = B(\mu_{n+1} - \mu_n) - B(\mu_n - \mu_{n-1})$$

$$M\ddot{\mu}_n = B(\mu_{n+1} + \mu_{n-1} - 2\mu_n) \quad \text{— WAVE EQUATION}$$

$$\mu = \mu_0 e^{i(\omega t - kx)} \quad \ni \quad \omega = 2\pi f;\ k = \frac{2\pi}{\lambda}$$

DIFFERENTIATE TWICE AND PLUG INTO EQUATION

$$\mu_n = \mu_0 e^{i(\omega t - kna)} \qquad x = na)$$

$$\mu_{n-1} = \mu_0 e^{i(\omega t - k(n-1)a)}$$

$$\mu_{n+1} = \mu_0 e^{i(\omega t - k(n+1)a)}$$

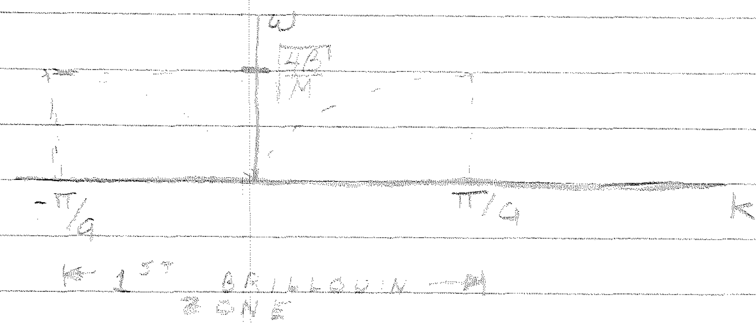
$$-\omega^2 M \mu_0 e^{i(\omega t - kna)} = B\mu_0 e^{i(\omega t - kna)}\left[e^{ika} + e^{-ika} - 2\right]$$

$$e^{ika} + e^{-ika} - 2 = \left(e^{\frac{ika}{2}} - e^{-\frac{ika}{2}}\right)^2$$

$$= -4\sin^2\frac{ka}{2}$$

$$\Rightarrow \omega^2 M = -4B\sin^2\frac{ka}{2} \Rightarrow \omega = \sqrt{\frac{4B}{M}}\sin\frac{ka}{2}$$

RELATION OF f & λ



SINGLE FREQ. WAVES:

PHASE SPEED: $V_p = f\lambda = \omega/k$

SPEED DECREASES FOR HIGHER FREQUENCIES

TRANSMISSION OF ENERGY FROM ONE POINT TO ANOTHER: GROUP VELOCITY

$$V_g = \frac{d\omega}{dk}$$

DIATONIC LATTICE

$2n-2$	$2n-1$	$2n$	$2n+1$
M	m	M	m

$\leftarrow 2a \rightarrow$

TWO D.E.'S

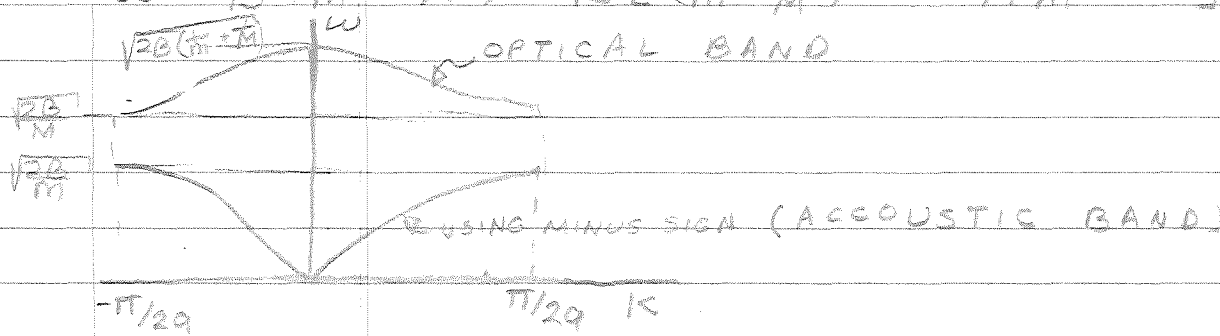
$$M\ddot{\mu}_{2n} = B(\mu_{2n+1} + \mu_{2n-1} - 2\mu_{2n})$$

$$m\ddot{\mu}_{2n+1} = B(\mu_{2n} + \mu_{2n+2} - 2\mu_{2n+1})$$

$$\Rightarrow \mu_{2n} = \xi e^{i(\omega t + 2nka)}$$

$$\mu_{2n+1} = \eta e^{i(\omega t + (2n+1)ka)}$$

$$\omega^2 = B\left(\frac{1}{m} + \frac{1}{M}\right) \pm B\left[\left(\frac{1}{m} + \frac{1}{M}\right)^2 - \frac{4\sin^2 ka}{Mm}\right]^{\frac{1}{2}}$$



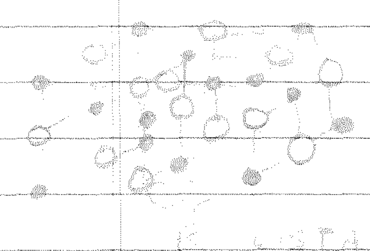
THE STRING OF ATOMS BEHAVES LIKE A SPRING WHEN ONE IS PUSHED

3-[illegible] (TUES)

IONIC CRYSTALS

A) LATTICE POTENTIAL ENERGY (E)

e.g. NaCl   Na ○ Cl ●



R DISTANCE THAT NEAREST NEIGHBORS

CUBE OF VOLUME R^3 CONTAINS $\frac{1}{2}$ Na AND $\frac{1}{2}$ Cl

SUPPOSE N ION PAIRS IN WHOLE SINGLE CRYSTAL

(N SODIUM, N CHLORINE)

VOLUME V OF WHOLE CRYSTAL:

$V = 2NR^3$

OTHER CRYSTALS: $V = CNR^3$

LATTICE POTENTIAL ENERGY

TWO IONS $\begin{cases} E = \underbrace{E_a(\text{ATTRACTIVE})}_{\text{COULOMB}} + \underbrace{E_r(\text{REPULSIVE})}_{\text{EXCLUSION}} \\ E_a = \dfrac{q_1 q_2}{4\pi\epsilon_0 r_{12}} \end{cases}$

ION # 1 (SODIUM IN CENTER)

$$E_{a1} = \frac{q_1 q_2}{4\pi\epsilon_0 r_{12}} + \frac{q_1 q_3}{4\pi\epsilon_0 r_{13}} + \frac{q_1 q_4}{4\pi\epsilon_0 r_{14}} + \ldots$$

$$E_{a1} = -\frac{e^2}{4\pi\epsilon_0 R}\left(\frac{6}{1} - \frac{12}{\sqrt{2}} + \frac{8}{\sqrt{3}} - \ldots\right)$$

INCLUDING ONLY THAT PART OF THE ATOM INSIDE CUBE:

$$E_{a1} = -\frac{e^2}{4\pi\epsilon_0 R}\left(\frac{3}{1} - \frac{3}{\sqrt{2}} + \frac{1}{\sqrt{3}} - \ldots\right)$$

CALLED EVJEN METHOD OF CUTTING OFF THE SERIES

$$E_c = \frac{-\alpha e^2}{4\pi\epsilon_0 R}$$

α: MODELING CONSTANT = 1.747 FOR NaCl

ION #1 EXCLUSION PRINCIPLE REPULSION

WE WORRY ABOUT NEAREST NEIGHBOR ONLY

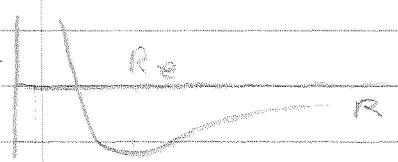
$$E_e = A/r^n$$

TOTAL P.E.; $E_1 = \frac{-\alpha e^2}{4\pi\epsilon_0 R} + \frac{A}{r^n}$

RECALL N ION PAIRS IN WHOLE CRYSTAL (2N IONS)

TOTAL ENERGY

$$E_T = N\left[\frac{-\alpha e^2}{4\pi\epsilon_0 R} + \frac{A}{R^n}\right]$$



@ T = 0°K, R = Re

$$\left.\frac{\delta E_T}{\delta R}\right|_{R=Re} = 0 = N\left[\frac{\alpha e^2}{4\pi\epsilon_0 Re^2} - \frac{nA}{Re^{n+1}}\right]$$

$$A = \alpha e^2 Re^{n-1}/4\pi\epsilon_0 n$$

$$E_T = N\left[\frac{-\alpha e^2}{4\pi\epsilon_0 R} + \frac{\alpha e^2 Re^{n-1}}{4\pi\epsilon_0 n R^n}\right]$$

$$= \frac{-N\alpha e^2}{4\pi\epsilon_0}\left[\frac{1}{R} - Re^{n-1}/nR^n\right]$$

@ T = 0°K R = Re

$$\Rightarrow E_{T_0} = \frac{-N\alpha e^2}{4\pi\epsilon_0 Re}\left[1 - \frac{1}{n}\right]$$

$\Rightarrow$ n IS RELATED TO COMPRESSIBILITY K

$$K = -\frac{1}{V}\frac{dV}{dP}$$

$$dW = p\,dV = -dE$$

$$\frac{dP}{dV} = -d^2E/dV^2$$

$$\frac{1}{K} = -V\,dP/dV = V\,d^2E/dV^2 \quad (1)$$

$$\frac{dE}{dV} = \frac{dE}{dR}\frac{dR}{dV} \quad \text{AND} \quad \frac{d^2E}{dV^2} = \frac{dE}{dR}\frac{d}{dV}\left(\frac{dR}{dV}\right) + \frac{d}{dV}\left(\frac{dE}{dR}\right)\left(\frac{dR}{dV}\right)$$

$$= \frac{dE}{dR}\frac{d^2R}{dV^2} + \frac{d^2E}{dR^2}\left(\frac{dR}{dV}\right)^2 \quad (2)$$

FROM (1) AND (2)

$$\frac{1}{K_0} = V\left[\cancel{\frac{dE}{dR}}\frac{d^2R}{dV^2} + \frac{d^2E}{dR^2}\left(\frac{dR}{dV}\right)^2\right]$$

$$= V\frac{d^2E}{dR^2}\left[\frac{dR}{dV}\right]^2$$

$$\frac{dV}{dR} = 3CNR^2$$

$$\frac{1}{K_0} = CNR_e^3 \frac{d^2E}{dR^2}\left[\frac{1}{9C^2N^2R_e^4}\right]$$

$$= \frac{1}{9CNR_e}\left(\frac{d^2E}{dR^2}\right)\Big|_{R=R_e}$$

$$\frac{d^2E}{dR^2}\Big|_{R=R_e} = \frac{N\alpha e^2}{4\pi\epsilon_0}\left[\frac{n-1}{R_e^3}\right]$$

$$\frac{1}{K_0} = \frac{1}{9CNR_e}\left[\frac{N\alpha e^2}{4\pi\epsilon_0}\left(\frac{n-1}{R_e^3}\right)\right]$$

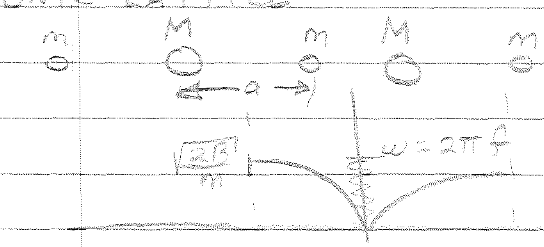
$$= \frac{\alpha e^2(n-1)}{36\pi C\epsilon_0 R_e^4}$$

n IS WHAT WE'LL SOLVE FOR; ALL OTHER CONSTANTS WE'LL KNOW

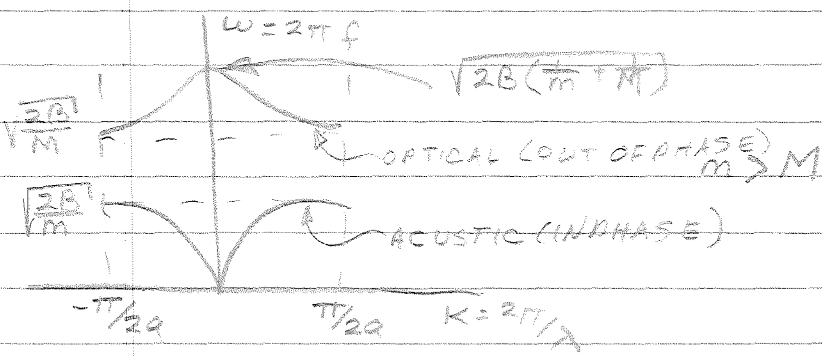
GO TO WEDNESDAY; PG. 11

3-24-72 (FRI) TEST ON MONDAY (SEC 3-4, 7)

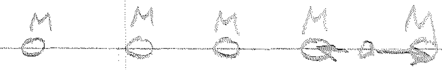
DIATONIC LATTICE

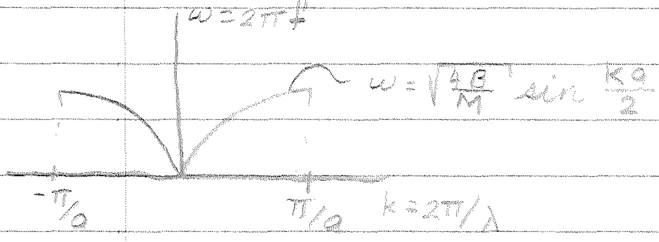


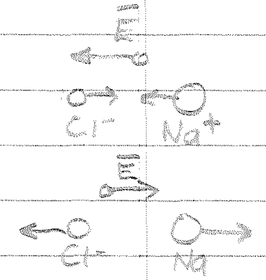
B = FORCE CONSTANT

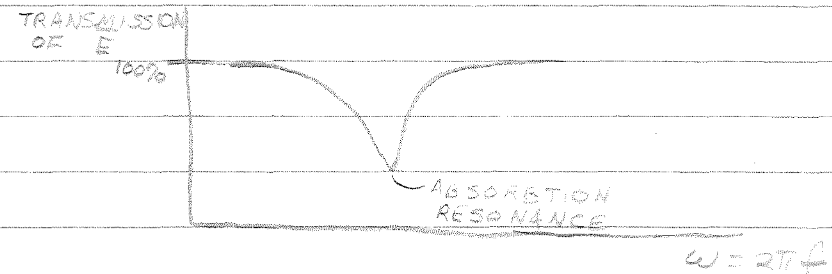


MONATONIC LATTICE

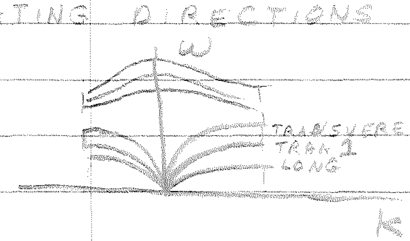






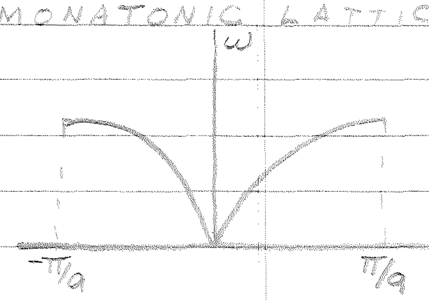


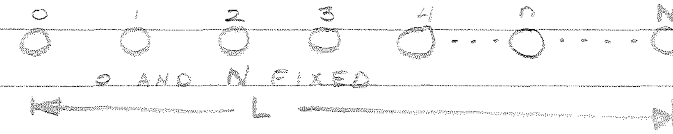
3 VIBRATING DIRECTIONS IN 3-D



$V_{ph} = \omega/k$

MONATONIC LATTICE - LONGITUDINAL VIBRATIONS





$u = u_0 e^{i\omega t} \sin kx$ (STANDING WAVE)

REAL PART

$\sin kL = \sin kNa = 0$

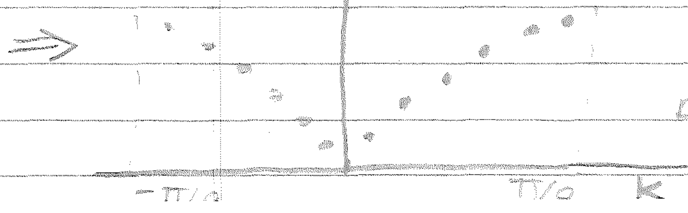
$\Rightarrow kL = kNa = \pi, 2\pi, 3\pi, \ldots$

$k = 2\pi/\lambda \Rightarrow L = \lambda/2$

$\Rightarrow k = \frac{\pi}{L}, \frac{2\pi}{L}, \frac{3\pi}{L}, \ldots, \frac{(n-1)\pi}{L}$

(@ $k = \frac{n\pi}{L}$, $u = 0$)

$\Rightarrow$



DISCRETE k AND ω!

REVIEW FOR TEST:

A) FORCES BETWEEN IONS

B) CRYSTAL STRUCTURE

(1) LATTICE, UNIT CELLS, BRAVAIS LATTICES,
LATTICE CONSTANTS

(2) MILLER INDICES

(3) SPACING 'TWIXT PLANES

(4) X-RAY DIFFRACTION DETERMINATION OF
UNIT CELL, LATTICE CONSTANS

C) IONIC CRYSTALS

(1) POTENTIAL ENERGY

(2) COMPRESSIBILITY AND n

(3) ELASTIC WAVES

(a) FREQ, WAVELENGTH, WAVE SPEEDS

(b) INFRARED ABSORBTION

(c) STANDING WAVE NODES

GO TO TUES (Pg 21)

3-29-72 (WED) DO 3-1 12-33

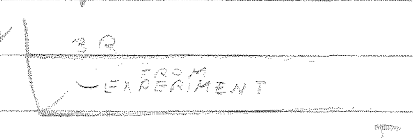
SPECIFIC HEAT OF SOLID

$C = \frac{\delta Q}{\delta T}$ (PER MOLE)

$C_v = \frac{\delta Q}{\delta T}\Big|_v = \frac{\delta U}{\delta T}\Big|_v$

FROM CLASSICAL CALCULATION; $U = 3RT$ (ANY ENERGY ALLOWED)

$C_v = 3R$



FROM QUANTUM MECHANICAL OSCILLATORS

$E = (n+\frac{1}{2})hf \quad ; \; n = 0, 1, 2, 3, \ldots$

EINSTEIN MODEL OF SOLID

(1) ALL ATOMS VIBRATE WITH SINGLE FREQUENCY f

(2) EACH OSCILLATOR IS 3 LINEAR HARMONIC OSCILLATORS (MUTUALLY $\perp$ VIBRATIONS)

(3) N ATOMS $\rightarrow$ 3N LINEAR OSCILLATORS

(4) BOLTZMANN DISTRIBUTION $\Leftarrow$ $U = 3N\bar{E}$ ($\bar{E}$ = AVERAGE)

$N_i \propto e^{-E_i/kT}$

$\bar{E} = \sum_i E_i e^{-E_i/kT} \Big/ \sum_i e^{-E_i/kT}$

$\bar{E} = \sum_{n=0}^{\infty} (n+\frac{1}{2})hf\, e^{-(n+\frac{1}{2})hf/kT} \Big/ \sum_{n=0}^{\infty} e^{-(n+\frac{1}{2})hf/kT}$

$$= \frac{e^{-\frac{1}{2}\frac{hf}{kT}} \sum_{n=0}^{\infty} (n+\frac{1}{2})hf\, e^{-nhf/kT}}{e^{-\frac{1}{2}hf/kT} \sum_{n=0}^{\infty} e^{-nhf/kT}}$$

$$= \frac{\frac{1}{2}hf \sum_{n=0}^{\infty} e^{-nhf/kT}}{\sum_{n=0}^{\infty} e^{-nhf/kT}} + \frac{\sum_{n=0}^{\infty} nhf\, e^{-nhf/kT}}{\sum_{n=0}^{\infty} e^{-nhf/kT}}$$

$$= \frac{1}{2}hf + \frac{hf e^{-hf/kT} + 2hf e^{-2hf/kT} + 3hf e^{-\frac{3hf}{kT}} + \ldots}{1 + e^{-hf/kT} + e^{-2hf/kT} + \ldots}$$

LET $x = -hf/kT$

$$\Rightarrow \bar{E} = \frac{1}{2}hf + hf\left(\frac{e^{x} + 2e^{2x} + 3e^{3x} + \ldots}{1 + e^{x} + e^{2x} + \ldots}\right)$$

LET $U = 1 + e^{x} + e^{2x} + e^{3x} + \ldots = \text{DEN} = \frac{1}{1 - e^{x}}$

~~$\Rightarrow \bar{E} = \frac{1}{2}hf + hf($~~

$$\frac{du}{dx} = e^{x} + 2e^{2x} + 3e^{3x} + \ldots = \text{NUMERATOR} =$$

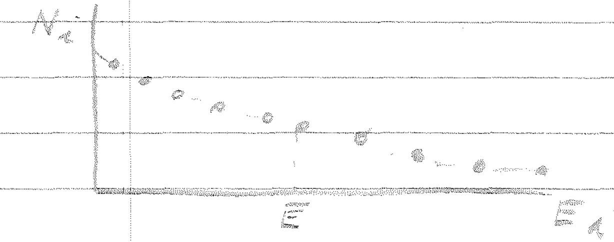
$$\frac{d}{dx}\left(\frac{1}{1-e^{+x}}\right) = +e^{+x}(1-e^{+x})^{-2}$$

$$\bar{E} = \frac{1}{2}hf + hf\,\frac{(1-e^{+x})^{-2}(+e^{+x})}{(1-e^{+x})^{-1}}$$

$$= \frac{1}{2}hf + \frac{e^{x}(1-e^{x})^{-2}}{(1-e^{x})^{-1}}\,hf$$

$$\therefore \bar{E} = \frac{1}{2}hf + hf\left[\frac{e^{x}}{1-e^{x}}\right] = \frac{1}{2}hf + hf\left[\frac{1}{e^{-x}-1}\right]$$

$$= \frac{1}{2}hf + hf\left(\frac{1}{e^{hf/kT}-1}\right)$$



TOTAL ENERGY

$$U = 3N \times \bar{E} = \frac{3}{2}Nhf + 3Nhf\left[\frac{1}{e^{hf/kT}-1}\right]$$

$$C_V = \left.\frac{\delta U}{\delta T}\right]_V = 3Nfh\frac{\delta}{\delta T}\left(e^{hf/kT}-1\right)^{-1}$$

$$= 3Nfh\left[(-1)\left(e^{hf/kT}-1\right)^{-2} e^{hf/kT}\left(-\frac{hf}{kT^2}\right)\right]$$

$$= 3N\left[\left(\frac{hf}{kT}\right)^2 e^{hf/kT}\Big/\left(e^{hf/kT}-1\right)^2\right]$$

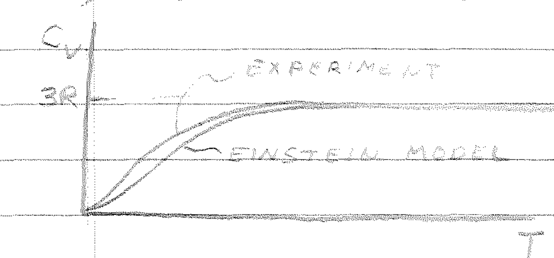
FOR 1 MOLE, $N = N_0$ = AVAGADRO'S #

$$\Rightarrow C_V = 3R\left[\left(\frac{hf}{kT}\right)^2 e^{hf/kT}\Big/\left(e^{hf/kT}-1\right)^2\right]$$

AS $T \to \infty$; $e^{hf/kT} \sim 1$

$$e^{hf/kT} - 1 \sim \frac{hf}{kT}\ ; \quad \lim_{T\to\infty} C_V = 3R$$

AS $T \to 0$; $C_V \to 3R\left(\frac{hf}{kT}\right)^2 e^{-hf/kT} \to 0$ (USING L'HOPITAL'S RULE)



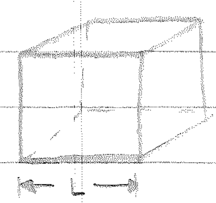
DEBYE MODEL

(1) 3N LINEAR HARMONIC OSCILLATORS

(2) MAXWELL DISTRIBUTION

(3) INSTEAD OF SINGLE VIBRATION FREQUENCY

a) ASSUMED FREQUENCIES PRESENT ARE STANDING WAVE FREQUENCIES OF CONTINUOUS MEDIUM



$L = n \, \lambda/2 \; ; \; n = 1, 2, 3, \ldots$

$f = v/\lambda$

b) ASSUMTION: ALL WAVES TRAVEL @ SAME SPEED (NON-DISPERSIVE)

$$\frac{\delta^2 u}{\delta^2 x} + \frac{\delta^2 u}{\delta y^2} + \frac{\delta^2 u}{\delta z^2} = \frac{1}{v^2}\frac{\delta^2 u}{\delta t^2}$$

FOR 1-DIMENSIONAL: (STANDING WAVE)

$$u = u_0 \sin\left(\frac{n_x \pi x}{L}\right) \cos 2\pi f t$$

FOR 3D

$$u = u_0 \sin\left(\frac{n_x \pi x}{L}\right) \sin\left(\frac{n_y \pi y}{L}\right) \sin\left(\frac{n_z \pi z}{L}\right) \cdot \cos 2\pi f t$$

TUES (2-29-72) PP 113-123

SPECIFIC HTS.

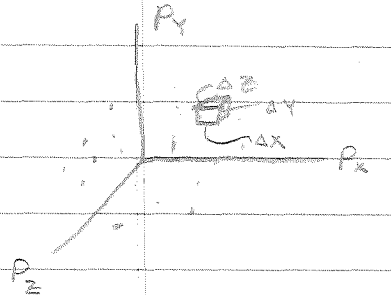
(1) CLASSICAL STATISTICAL MECHANICS

TO DETERMINE EQUALIBRIUM ENERGY DISTRIBUTION

MOMENTUM SPACE

FREE PARTICLES

ENERGY DEPENDS ONLY ON MOM.



IF PARTICLE IS NOT FREE:

$E(P_X, P_Y, P_Z, X, Y, Z)$; CONSERVATIVE SYSTEM

6-DIMENSIONAL GRAPH; PHASE SPACE, WITH BOXES OF $dp_x\, dp_y\, dp_z\, dx\, dy\, dz$

DISTRIBUTION OF PARTICLES AMONG CELLS IN PHASE SPACE WILL GIVE ENERGY DISTRIBUTION

#1	#2	#3	#4	#5
N_1	N_2	N_3	N_4	N_5

N = TOTAL PARTICLES

EQUALIBRIUM DISTRIBUTION = MOST PROBABLE DISTRIBUTION OF PTS. AMONG CELLS

EXAMPLE: 2 BOXES; 4 PARTICLES

a) ALL 4 IN A CELL (ONE WAY)

b) 3 IN A 1 IN B (4 WAYS)

c) 2 IN A, 2 IN B (6 WAYS)

$WAYS = N!/N_1!\,N_2!\,N_3!\ldots$

PROBABILITY OF A DISTRIBUTION OF PTS AMONG CELLS IS: $P \propto$ WAYS

WHICH DISTRIBUTION HAS MAXIMUM PROBABILITY WITH RESTRICTIONS:

$N = N_1 + N_2 + \ldots = $ CONSTANT

$E = N_1E_1 + N_2E_2 + \ldots = $ CONSTANT

LEGRANGES MULTIPLIERS:

$N_i \propto e^{E_i/nt}$; MAXWELL-BOLTZMAN DISTRIBUTION

$E_1, E_2, E_3, \dots \Rightarrow$ DISCRETE ENERGIES (QUANTUM)

N_i = # PARTICLES WITH ENERGY E_i

CONTINUOUS ENERGY DISTRIBUTION

BOXES HAVE "VOLUME" IN PHASE SPACE:

$$d\Omega = dp_x\, dp_y\, dp_z\, dx\, dy\, dz$$

$$\Rightarrow dN \propto e^{-E/kT} d\Omega \quad \text{(MAXWELL-BOLTZMAN)}$$

EXAMPLE: CLASSICAL VIBRATING ATOM $\Rightarrow$ NO E RESTRICTIONS

FRACTION OF THE PARTICLES @ P ($p_x p_y p_z$) AND POSITION X, Y, Z IN PHASE SPACE IN $d\Omega$

$$= \frac{dN}{N} = e^{-E/kT} d\Omega \Big/ \int_{-\infty}^{\infty} e^{-E/kT} d\Omega$$

$$= \frac{p_x^2 + p_y^2 + p_z^2}{2m} + \frac{1}{2}\beta(x^2 + y^2 + z^2)$$

$$\bar{E} = \frac{\int E\, dN}{N} = \frac{\int E\, e^{-E/kT} d\Omega}{\int e^{-E/kT} d\Omega} = 3kT$$

TOTAL E ON N VIBRATING ATOMS:

$U = 3NkT$

FOR ~~1~~ GRAMS MOLE

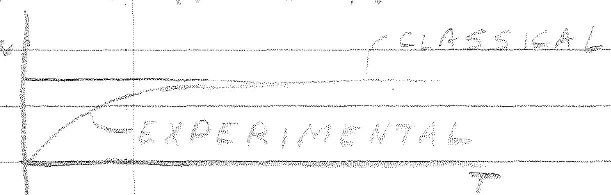
$U = 3N_0kT = 3RT$

N_0 = AVAGADRO'S NUMBER

R = IDEAL GAS CONSTANT

SPECIFIC HT/PER MOLE

$$C_V = \left.\frac{\delta Q}{\delta T}\right|_V = \left.\frac{\delta U}{\delta T}\right|_V = 3R = 5.96 \text{ CALORIES/MOLE } {}^\circ K$$



VIBRATING PARTICLE CAN HAVE ENERGIES

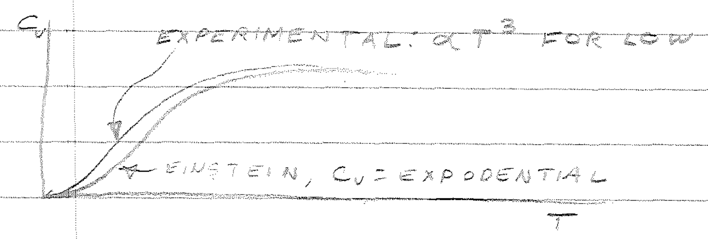
$$E = (n + \tfrac{1}{2})hf \quad ; \; n = 0, 1, 2, 3, \dots$$

TO WED (Pg 18)

4-3-72 (MON)

LATTICE VIBRATION → SPECIFIC HT OF SOLID

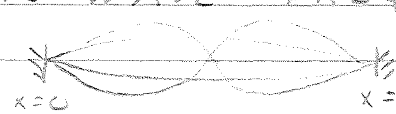
(1) EINSTEIN MODEL



(2) DEBYE MODEL

FREQUENCIES ARE CONTINUOUS MEDIUM

STANDING WAVE FREQUENCIES



$$\frac{\delta^2 u}{\delta x^2} + \frac{\delta^2 u}{\delta y^2} + \frac{\delta^2 u}{\delta z^2} = \frac{1}{V^2}\frac{\delta^2 u}{\delta t^2}$$

$$\mu = \mu_0 \sin\left(\frac{n_x \pi x}{\ell}\right)\sin\left(\frac{n_y \pi y}{\ell}\right)\sin\left(\frac{n_z \pi z}{\ell}\right)\cos 2\pi f t;\ n_x, n_y, n_z = 1, 2, 3, \ldots$$

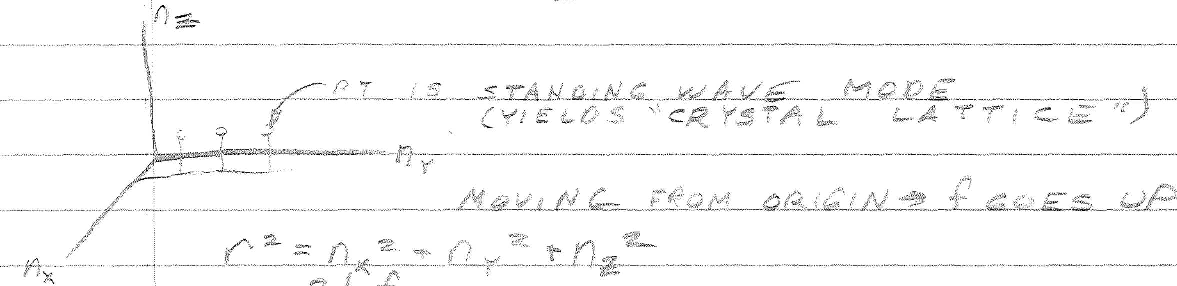
PLUGGING BACK INTO D.E.:

$$-\left(\frac{n_x \pi}{\ell}\right)^2\mu - \left(\frac{n_y \pi}{\ell}\right)^2\mu - \left(\frac{n_z \pi}{\ell}\right)^2\mu = \frac{1}{V^2}\left[(-4\pi^2 f^2)\mu\right]$$

$$\left(\frac{\pi}{\ell}\right)^2(n_x^2 + n_y^2 + n_z^2) = 4\pi^2 f^2 / V^2$$

STANDING WAVE FREQUENCIES:

$$f = \frac{V}{2\ell}\sqrt{n_x^2 + n_y^2 + n_z^2}$$



MOVING FROM ORIGIN → f GOES UP

$$r^2 = n_x^2 + n_y^2 + n_z^2$$

$$\Rightarrow R = \frac{2Lf}{V}$$

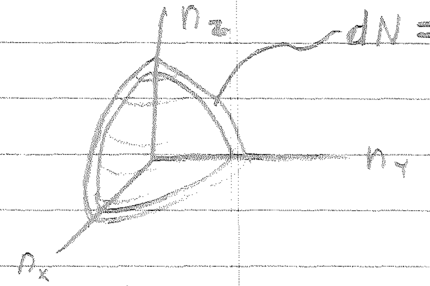
$$dR = \frac{2L}{V}\,df$$

TO GET # OF VIBRATION MODES 'TWIXT f AND $f + df = dN$

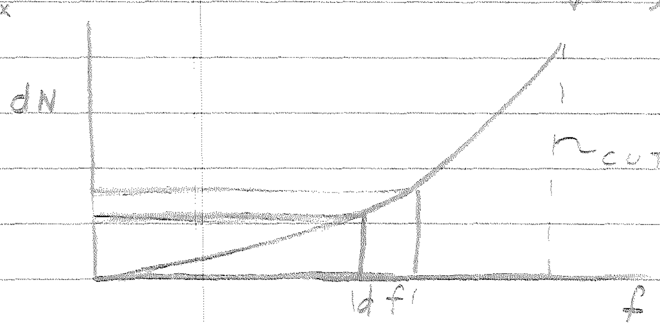
= (COUNT # OF PTS 'TWIXT R & R+dR)

VOLUME 'TWIXT R & R+dR (FLIP OVER)

WILL GIVE A SPHERE SHELL



$$dN = \frac{1}{8}(4\pi R^2)\,dR$$
$$= \frac{\pi}{2} R^2 dR$$
$$= \frac{\pi}{2}\left(\frac{4\ell^2 f^2}{V^2}\right)\left(\frac{2\ell}{V}\,df\right)$$
$$= \frac{4\pi\ell^3}{V^3} f^2 df$$
$$= \frac{4\pi \mathbb{V}}{V^3} f^2 df \ni \ell^3 = \text{CUBE VOLUME} = \mathbb{V}$$



WITH
TWO TRANSVERSE VIB. W/ VELOCITY V_T
ONE LONGITUDINAL VIB. W/ VELOCITY V_ℓ

$$\Rightarrow dN = 4\pi\mathbb{V}\left(\frac{2}{V_t^3} + \frac{1}{V_\ell^2}\right) f^2 df$$
$$3N = \int_0^{f_d} dN$$
$$= 4\pi\mathbb{V}\left(\frac{3}{V_t^3} + \frac{1}{V_\ell^2}\right)\int_0^{f_d} f^2 df$$

$$\therefore f_0 = \left[\frac{9}{4\pi}\,\frac{N}{\mathbb{V}}\left(\frac{2}{V_t^3} + \frac{1}{V_\ell^3}\right)^{-1}\right]^{1/3}$$

LET EACH OSCILLATOR HAVE ENERGY EQUAL TO AVERAGE ENERGY OF EINSTEIN'S OSCILLATORS:

$$\bar{E} = \frac{hf}{e^{hf/kT} - 1}$$

TOTAL ENERGY: $U = \int_0^{f_0} E\,dN$

$$= \int_0^{f_0}\left(\frac{hf}{e^{hf/kT} - 1}\right) dN$$

$$U = 4\pi\mathbb{V}\left(\frac{2}{V_t^3} + \frac{1}{V_\ell^3}\right)\int_0^{f_0}\frac{hf^3 df}{e^{hf/kT} - 1}$$

SUBSTITUTE $\left(\frac{2}{V_t^3} + \frac{1}{V_\ell^3}\right)$ FROM EXPRESSION FOR f_0

LET $x = hf/kT$ AND $x_0 = hf_0/kT$

$$\Rightarrow 9N\left(\frac{kT}{hf_0}\right)^3 kT\int_0^{x_0}\frac{x^3 dx}{e^x - 1} = U$$

FOR HI T; $U \cong 9N\left(\frac{kT}{hf_0}\right)^3\int_0^{x_0}\frac{x^3 dx}{(x+1) - x}$; $e^x \cong 1 + x$ FOR SMALL x

$$\cong 3NkT = 3RT \ \frac{\text{JOULES}}{\text{MOLE}}$$

$$\rightarrow c_v = \left.\frac{\delta U}{\delta T}\right]_v = 3R$$

<u>LOW TEMP:</u>

$$U \doteq 9T\left(\frac{kT}{hf_0}\right)^3 kT \int_0^{x_0} \frac{x^3\,dx}{e^x - 1}$$

LOW $T \Rightarrow$ HIGH $x_0 \cong \infty$

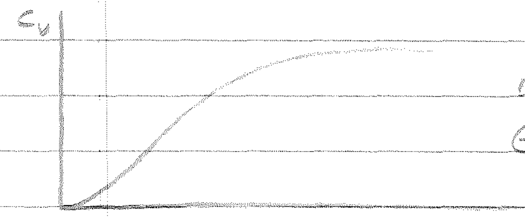
$$\Rightarrow U \cong 9T\left(\frac{kT}{hf_0}\right)^3 kT \int_0^{\infty} \frac{x^3\,dx}{e^x-1}$$

$$\int_0^{\infty} \frac{x^3\,dx}{e^x-1} = \pi^4/15$$

$$\therefore U \cong \frac{3}{5}\pi^4 NkT\left(\frac{T^3}{\Theta_D^3}\right) \qquad \ni \Theta_D = \frac{hf_0}{k}$$

Θ_D = DEBYE TEMPERATURE

$$C_v = \frac{\delta U}{\delta T}\Big]_v = \frac{R}{5}\pi^4 R\left(\frac{T}{\Theta_D}\right)^3$$



DEBYE HAS GOOD FIT: CHOOSE Θ_D TO MAKE CURVE FIT THE EXPERIMENT. Θ_D (BEGINS ON THE SUBSTANCE)

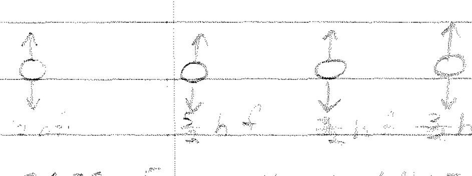
4-4-72 (TUES) TEST NEXT WEDNESDAY pp. 147-59

SPECIFIC HEAT: C_v

(1) INSULATORS: $C_v = \left(\frac{\delta U_{VIB}}{\delta T}\right)_v$

(2) METALS: $C_v = \left[\left(\frac{\delta U_{VIB}}{\delta T}\right) + \left(\frac{\delta U_{ELEC}}{\delta T}\right)\right]_v$

$= (C_v)_{VIB} + (C_v)_{ELEC}$



← VIBRATING @ FREQ: f

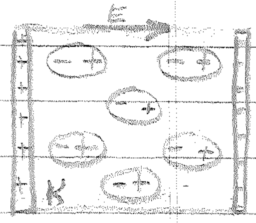
$\frac{1}{2}hf$ $\quad \frac{5}{2}hf$ $\quad$ [illegible] $\quad \frac{3}{2}hf$ $\qquad \therefore E = (n + \frac{1}{2})hf$

MAY PASS E ONLY IN UNITS OF $E = hf$ (VIBRATIONAL ELEMENT)

hf = PHONON

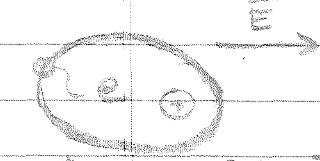
$P = \hbar k \ni k = \frac{2\pi}{\lambda}$; P = PHONON VIBRATION

DIELECTRICS



- POLARIZATION

a) ELECTRONIC POLARIZATION (SHIFT e^- ORBITS RELATIVE TO NUCLEUS)

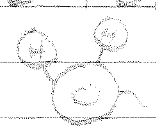


b) Na^+ $\oplus \longrightarrow$ $\longleftarrow \ominus$ Cl $\xrightarrow{E}$

IONIC POLARIZATION

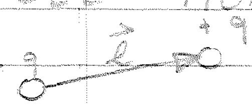
c) ORIENTATIONAL POLARIZATION (REORIENTATION OF PERMANENT DIPOLE ON $\vec{E}$)

WATER:



DEFINITIONS:

(1) DIPOLE MOMENT; $\vec{p} = q\vec{l}$



(2) POLARIZATION; $\vec{P} = \sum_i \vec{p}_i / V$ = DIPOLE MOMENT/UNIT VOLUME

(3) DISPLACEMENT; $\vec{D} = \epsilon_0 \vec{E} + \vec{P}$ (MKS)

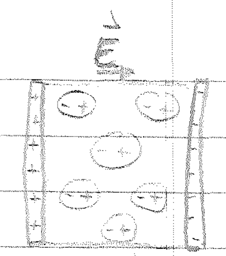
$\vec{D} = \vec{E} + 4\pi\vec{P}$ (CGS)

DIELECTRIC DECREASES $\vec{E}$ IF CHARGE ON PLATES IS THE SAME

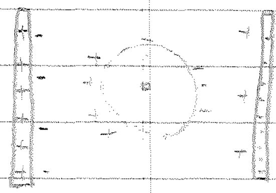
(4) DIELECTRIC CONSTANT; K

$\vec{D} = K\epsilon_0\vec{E} = \epsilon_0\vec{E} + \vec{P}$

$\Rightarrow K = 1 + \frac{P}{\epsilon_0 E}$



E_{loc} = LOCAL FIELD @ POSITION OF ATOM DUE TO OTHER CHARGES



E_1 = E FIELD @ PT. DUE TO PLATES

E_2 = E FIELD @ PT. DUE TO OUTSIDE SURFACE POLARIZATION CHARGE

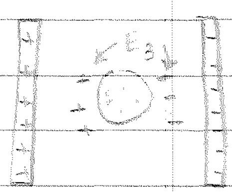
E_3 = E FIELD DUE TO CHARGE ON CAVITY SURFACE

E_4 = E FIELD INSIDE THE CAVITY

$$\Rightarrow \vec{E}_{loc} = \underbrace{\vec{E}_1 + \vec{E}_2}_{\vec{E}} + \vec{E}_3 + \vec{E}_4 = \vec{E} + \vec{E}_3 + \vec{E}_4$$

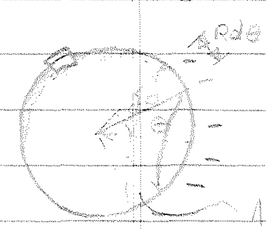
4-5-72 (TUES)

POLARIZATION IN A DIELECTRIC



E_4 DUE TO INDIVIDUAL DIPOLES

$E_{loc} = E + E_3 + E_4$



$$-\oint \vec{P} \cdot d\vec{S} = q_{pol}\text{ (ENCLOSED)}$$
$$= \sigma_p \, dS = -(P\cos\theta)\, dS$$
$$\Rightarrow \sigma_p = -P\cos\theta$$

AREA: $R\,d\theta\,2\pi R\sin\theta$

$$dq = \sigma(2\pi R^2 \sin\theta\, d\theta)$$

$$dE_3 = \frac{-1}{4\pi\epsilon_0}\frac{dq}{r^2}\cos\theta$$

$$\Rightarrow E_3 = \frac{-1}{4\pi\epsilon_0}\int \frac{dq}{r^2}\cos\theta$$
$$= \frac{P}{2\epsilon_0}\int_0^\pi \cos^2\theta \sin\theta\, d\theta$$
$$= -\frac{P}{2\epsilon_0}\frac{\cos^3\theta}{3}\Big|_0^\pi$$
$$= \frac{P}{3\epsilon_0}$$

$$\therefore E_{loc} = E + \frac{P}{3\epsilon_0} + E_4$$

1) FOR CUBIC LATTICE OF SAME ATOM; $E_4 = 0 \Rightarrow E_{loc} = E + \frac{P}{3\epsilon_0}$

2) SOME OTHER LATTICE; $E_4 \neq 0 \Rightarrow E_{loc} = E + \gamma_j P$

ATOM IN E FIELD (E_{loc})

$\xrightarrow{E}$ $\Rightarrow$ $- +$

ATOMIC POLARIZABILITY; $\alpha_j = \frac{p}{E_{loc}}$ p = DIPOLE MOMENT

CUBIC LATTICE OF IDENTICAL ATOMS

$$E_{loc} = E + P/3\epsilon_0 \qquad \left.\begin{array}{l}\vec{D} = K\epsilon_0\vec{E} \\ \vec{D} = \epsilon_0\vec{E} + \vec{P}\end{array}\right\} K = 1 + \frac{P}{3\epsilon_0}$$

$$K = 1 + \frac{P}{\epsilon_0 E} \Rightarrow P = (K-1)\epsilon_0 E$$

$$E_{loc} = E + (K-1)\frac{E}{3}$$

$$= \left(\frac{K+2}{3}\right)E$$

$$K - 1 = \frac{P}{\epsilon_0 E_{loc}}\left(\frac{3}{K+2}\right)$$

$$\frac{K-1}{K+2} = \frac{P}{3\epsilon_0 E_{loc}} \Rightarrow \text{CLAUSUIS-MOSSATI EQUATION}$$

N ATOMS PER UNIT VOLUME

$$\alpha = 10^{-40}\ m^3$$

He	.20	K_1^{4}	0.02
He	.39	C_0^4	0.42

IONIC POLARIZABILITY

APPLY FIELD E

SHIFT X OF X IONS RELATIVE TO NEGATIVE IONS

DIPOLE MOMENT $eE_{loc} = \beta X$

$$X = eE_{loc}/\beta$$

$$P_{ionic} = NeX \quad \text{(IONIC)}$$

$$= Ne^2 E_{loc}/\beta$$

$$\frac{K-1}{K+2} = \frac{P}{3\epsilon_0 E_{loc}} = \frac{N\alpha_1 E_{loc} + N\alpha_2 E_{loc} + Ne^2 E_{loc}/\beta}{3\epsilon_0 E_{loc}}$$

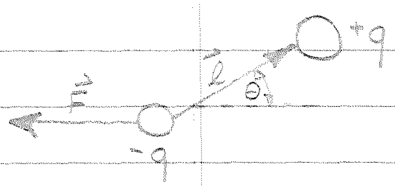
$$= \frac{N}{3\epsilon_0}\left[\alpha_1 + \alpha_2 + \frac{e^2}{\beta}\right]$$

$$\omega = \sqrt{\beta/m}$$

4-7-72 (FRI)

ORIENTATIONAL POLARIZATION-ALIGNMENT OF PERMANENT DIPOLES

WITH ELECTRIC FIELD PRESENT, FIELD TENDS TO LINE ~~TO LINE~~ UP DIPOLES, WHILE INTERACTIONS 'TWIXT THE DIPOLES THEMSELVES TEND TO RANDOMIZE DIRECTION

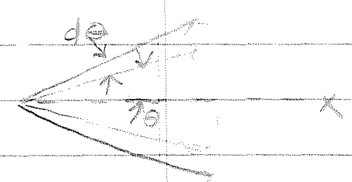


$$U = -\vec{p}\cdot\vec{E} = -pE\cos\theta$$

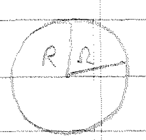
$$\bar{U} = \frac{1}{N}\int U\,dN$$

$$= \frac{-\int pE\cos\theta\, e^{pE\cos\theta/kT}\,d\Omega}{\int e^{pE\cos\theta/kT}}$$

$$\ni e^{-U/kT} = e^{pE\cos\theta/kT}$$



$d\Omega$ IS THE SOLID ANGLE 'TWIXT θ AND $\theta + d\theta$



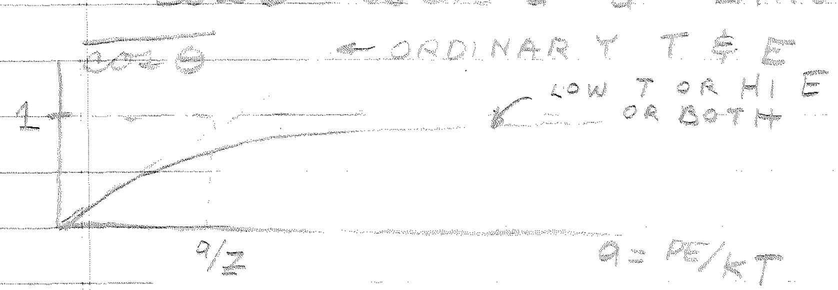
$$\Omega = \frac{\text{AREA SUBT. ON SPHERE}}{R^2}$$

$$\Rightarrow pE\,\overline{\cos\theta} = \frac{\int_0^\pi pE\cos\theta\, e^{pE\cos\theta/kT}\, 2\pi\sin\theta\, d\theta}{\int_0^\pi e^{pE\cos\theta/kT}\, 2\pi\sin\theta\, d\theta}$$

NOW $dx = -\sin\theta\, d\theta$; $x = \cos\theta$; $a = pE/kT$

$$\Rightarrow \overline{\cos\theta} = \frac{-\int_1^{-1} x e^{ax}\,dx}{-\int_1^{-1} e^{ax}\,dx} = \frac{e^a + e^{-a}}{e^a - e^{-a}} - \frac{1}{a}$$

$$\overline{\cos\theta} = \coth a - \frac{1}{a} = \text{LANGEVIN FUNCT.}$$



FOR NORMAL T AND E $a \ll 1$

$\overline{\cos\theta} = a/3$ (EXP IN SERIES)

$P = Np\,\overline{\cos\theta}$ ∋ N = NUMBER OF DIPOLES PER UNIT VOLUME

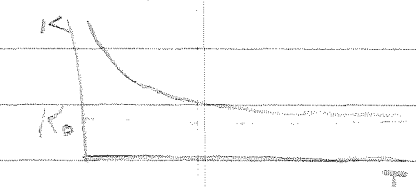
$= Np\,\frac{pE}{3kT} = Np^2E/3kT$

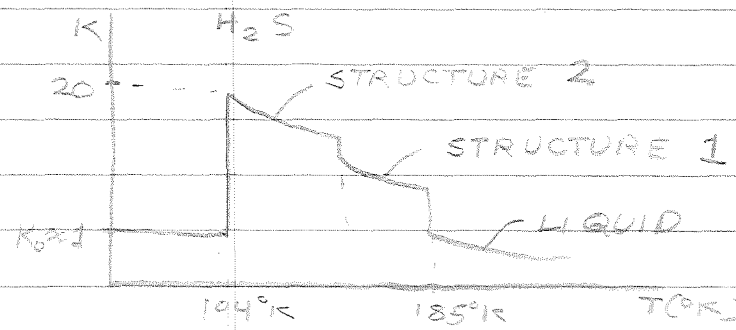
$K = 1 + \frac{P}{\epsilon_0 E}$

$= 1 + Np^2/3\epsilon_0 kT$

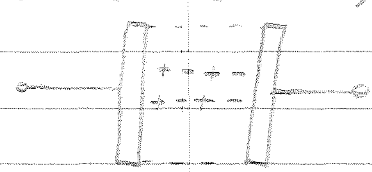
IF OTHER POLARIZATION BESIDES DIPOLE ORIENTATION

$K = K_0 + C/T$ (CURIE LAW)

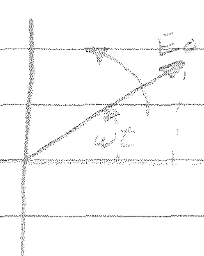




4-10-72 (MONDAY)



ALTERNATING ELECTRIC FIELDS (DIELECTRIC)



$E = E_0 e^{i\omega t}$

$$\Sigma F = m\frac{d^2x}{dt^2} = qE_0 e^{i\omega t} - \beta x - m\gamma\frac{dx}{dt}$$

β = RESTORING COEFFICIENT

m = MASS

γ = FUDGE FACTOR

$m\gamma\frac{dx}{dt}$ = RADIATION LOSS

$$\Rightarrow \frac{d^2x}{dt^2} + \frac{\beta}{m}x + \gamma\frac{dx}{dt} = \frac{q}{m}E_0 e^{i\omega t}$$

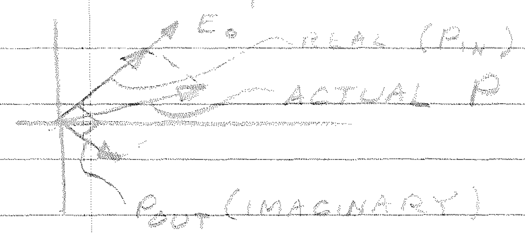
$$\frac{d^2x}{dt^2} + \gamma\frac{dx}{dt} + \omega_0^2 x = \frac{q}{m}E_0 e^{i\omega t}$$

$\checkmark$ MAGIC

$$x = \frac{q}{m}\left[\frac{E_0 e^{i\omega t}}{\omega_0^2 - \omega^2 + i\gamma\omega}\right] = \frac{qE_0}{m} e^{i\omega t}\left[\frac{\omega_0^2 - \omega^2 - i\gamma\omega}{(\omega_0^2-\omega^2)+\gamma^2\omega^2}\right]$$

$$= \frac{qE_0}{m} e^{i\omega t}\left\{\left[\frac{\omega_0^2-\omega^2}{(\omega_0^2-\omega^2)+\gamma^2\omega^2}\right] - i\left[\frac{\gamma\omega}{(\omega_0^2-\omega^2)+\gamma^2\omega^2}\right]\right\}$$

$$p = qx \Rightarrow P = NqX = \frac{Nq^2E_0}{m} e^{i\omega t}$$



FOR A SLOWLY VARYING FIELD ($\omega << \omega_0$)

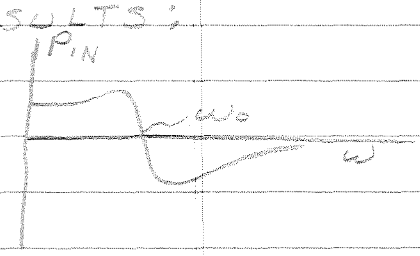
$$P_{IN} = \frac{Nq^2E_0}{m} e^{i\omega t}\left(\frac{1}{\omega^2}\right) ; \gamma^2\omega^2 \text{ NEGLIGIBLE}$$

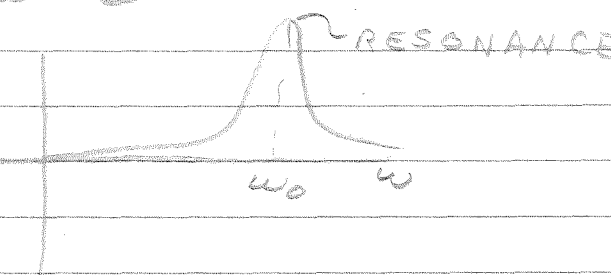
$$P_{OUT} = 0$$

NEAR $\omega = \omega_0$

$$P_{IN} = 0 ; P_{OUT} = \frac{Nq^2E_0}{m\gamma\omega} e^{i\omega t}$$

RESULTS:





@ $\omega >> \omega_0$

$$P_{IN} = \frac{Nq^2 E_0 e^{i\omega t}}{m} \left[\frac{-\omega^2}{\omega^4 + \gamma^2 \omega^2} \right]$$

HEADS TOWARD ZERO AFTER HUMP AFTER ω_0

$P_{OUT} \Rightarrow$ HEADS TOWARD ZERO

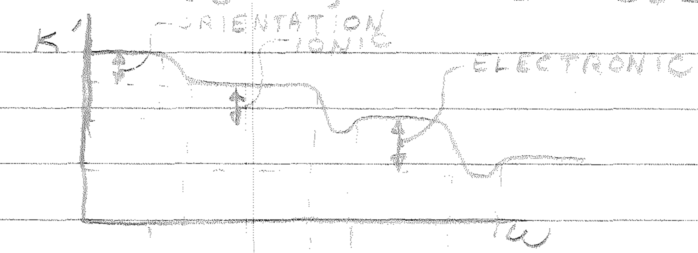
$$\text{POWER} = \frac{dw}{dt} = FV$$

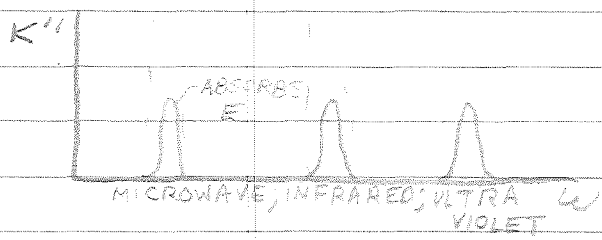
POWER INPUT MAXIMUM @ RESONANCE; $\omega = \omega_0$

E_0 @ MAX WHEN $X=0$, SINCE VELOCITY

V IS MAX @ $X=0$

$$K = 1 + \frac{P}{\epsilon_0 E} \; ; \; K' = 1 + \frac{P_{IN}}{\epsilon_0 E} \; ; \; K'' = 1 + \frac{P_{OUT}}{\epsilon_0 E}$$

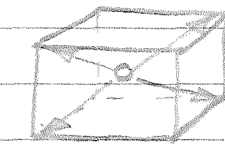




4-11-72 (TUESDAY)

FERRO-ELECTRICITY:

INVERSION CENTER OF SYMMETRY
-ALL POINTS INVERTED THRU
INVERSION CENTER



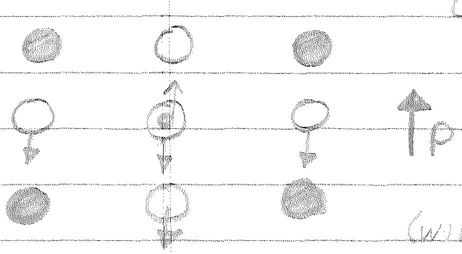
EX

FERRO-ELECTRICITY

1) UNIT CELLS HAVE NO INVERSION CENTER OF SYMMETRY
2) ALTERNATE POSITIONS FOR SOME ATOMS IN UNIT CELLS
3) DIPOLE IN ONE CELL HAS STRONG ENOUGH FIELD TO PRODUCE SIMILAR DIPOLE IN NEXT, ETC.
(CO-OPERATIVE PHENOMENON)

EX) $BaTiO_3$

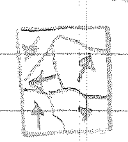
● Ba^{+2}
• Ti^{+4}
○ O^{-2}



Ti^{+4} OFF CENTER BY .06 Å
O^{-2} .09 Å
TETRAGONAL 278-393°K
(WILL CHANGE FROM CUBIC IN ABOVE TEMPERATURE CHANGE)

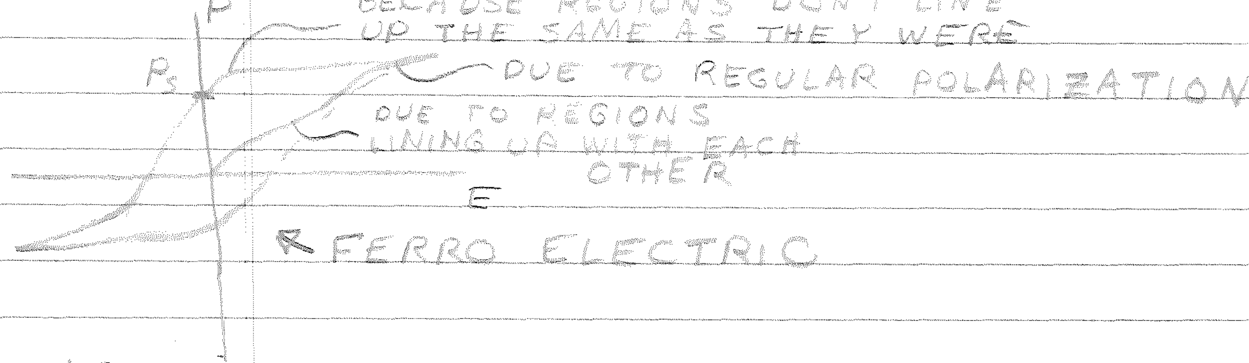
→ POLARIZATION WITH ALL DIPOLE MOMENTS IN A GIVEN REGION OF CRYSTAL (DOMAIN) IN THE SAME DIRECTION)

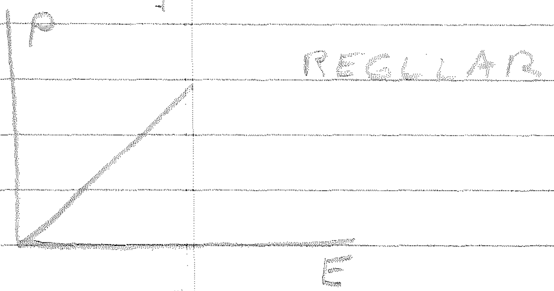
FOR $BaTiO_3$ (SINGLE CRYSTAL)



NO APPLIED E FIELD

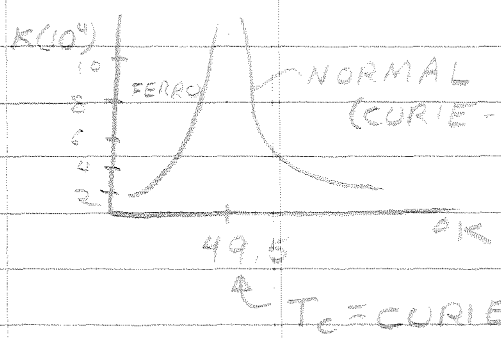
APPLYING $\vec{E}$ FIELD





$$K = 1 + \frac{P}{\epsilon_0 E}$$
$$= 1 + \frac{1}{\epsilon_0} \left.\frac{dP}{dE}\right|_{E=0}$$

TRIGLYANE SULPHATE



$$K = K_0 + \frac{C}{T - T_c}$$

TEST 2

I) SPECIFIC HT. OF INSULATORS

(NO SPECIFIC QUESTIONS ON STATISTICS)

1) EINSTEIN MODEL

MODEL, DERIVATION OF C_V, COMARISON W/EXPERIMENT

2) DEBYE MODEL

3) PHONON - PACKET OF VIBRATIONAL ENERGY

II) DIELECTRICS

1) DEFINITIONS OF $\vec{p}, \vec{P}, \vec{D}, \kappa, \alpha$

2) TYPES OF POLARIZATION

3) LOCAL FIELD @ ATOMIC POSITION

(DUE TO OTHER DIPOLES AND CHARGES)

4) CLAUSUIS - MESOTTI EQUATION

(DERIVATION, USE IN FINDING α)

5) IONIC POLARIZATION

6) ORIENTATIONAL POLARIZATION

(DERIVATION, DEPENDENCE OF P ON E & T)

7) DIELECTRIC IN ALTERNATING FIELD

8) FERRO-ELECTRICS

4-14 (FRI)

MAGNETIC PROCESSES

IF APPLY MAGNETIC FIELD OF INTENSITY $\vec{H}$ TO A MATERIAL → INDUCED MAGNETIZATION $\vec{M}$

$\vec{M} = \sum P_m / V$

$= \mu \vec{H} = \mu_0 \vec{H} + \vec{M}$; $\vec{B}$ = MAGNETIC INDUCTION

$= (\mu_0 + \chi)\vec{H}$; $\chi = \frac{M}{H}$ = MAGNETIC SUSCEPTIBILITY

MAGNETIC MOMENTS

1) ORBITAL MAGNETIC MOMENT (CIRCLE)

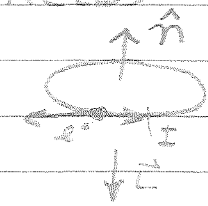
$\vec{P}_m = I A \hat{n}$

$\vec{P}_m = \frac{ev}{2\pi R}(\pi R^2)\hat{n}$

$= \frac{evR}{2}\hat{n}$

$= \left(\frac{-e}{2m}\right)(-mvr\hat{n})$

$= \left(\frac{-e}{2m}\right)\vec{L}$ → $\vec{L}$ = ORBITAL ANGULAR MOMENTUM → TRUE FOR ANY ORBIT



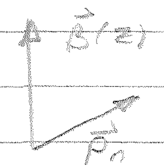
2) SPIN MAGNETIC MOMENT:

$\vec{P}_s = -g\left(\frac{e}{2m}\right)\vec{S}$ → $\vec{S}$ = SPIN ANGULAR MOMENTUM

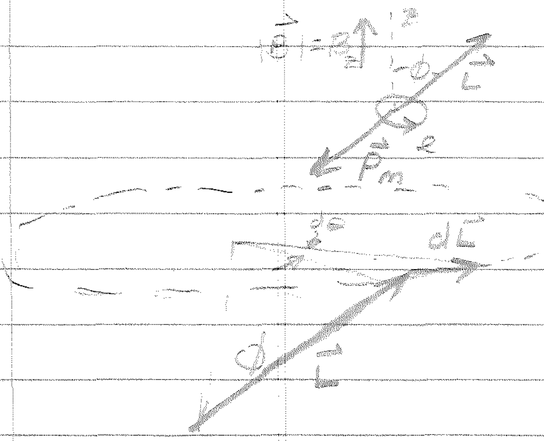
APPLY MAGNETIC FIELD

$\vec{\tau} = \vec{P} \times \vec{B}$

$U = -\vec{P}_m \cdot \vec{B}$



DIAMAGNETISM DUE TO LARMOR PRECESSION OF ELECTRON ORBIT



TORQUE INTO PAPER

$F = \delta P / \delta t$; $\tau = \delta L / \delta t = \vec{P}_m \times \vec{B}$

$\vec{\tau} = \frac{d\vec{L}}{dt} = \vec{p}_m \times \vec{B}$

$= -\left(\frac{e}{2m}\right) \vec{L} \times \vec{B}$

$d\vec{L} = \boxed{\left(\frac{e}{2m}\right) \vec{B} \times \vec{L}}\, dt$

ω_L = LAMORE PRECESSON FREQUENCY (RAD/SEC)

$\omega_L = d\theta/dt$

$d\theta = \omega_L dt \Rightarrow d\theta = \omega_L dt = \frac{dL}{L \sin\phi}$

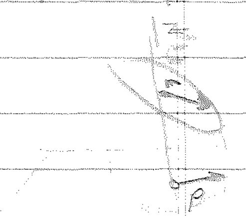
$|d\vec{L}| = \omega_L L \sin\phi\, dt = |\vec{\omega}_L \times \vec{L}|\, dt$

SOVING FOR ω_L:

$\omega_L = \left(\frac{e}{2m}\right) \vec{B}$ $\Rightarrow$ LAMOR PRECISION FREQ.

INDUCED ANGULAR MOMETUM $\rightarrow$ DIAMAGNETIC EFFECT (ALL IN ELECTRONS ORBIT)

$\rightarrow L_{IND} = m\omega_L \rho^2$



$IND\ (\vec{p}_m) = -\frac{e}{2m} m\omega_L \rho^2$

$\rightarrow$ SPHRERICAL RADIUS $= \overline{r}$

$\overline{r^2} = \overline{x^2} + \overline{y^2} + \overline{z^2} = 3\overline{x^2}$

$\overline{\rho^2} = \overline{x^2} + \overline{y^2} = 2\overline{x^2}$

$\overline{\rho^2} = \frac{2}{3} \overline{r^2}$

$\rightarrow p_{IND} = -Z\left(\frac{e}{2m}\right) m\omega_L \left(\frac{2}{3} \overline{r^2}\right)$

ASSUME N ATOMS/VOLUME

$M = N p_{ind}$ $\quad B = \mu_0 H$

$\chi = M/H = N p_{ind}/H$

$\chi_d = -\mu_0 N Z \left(\frac{e^2}{6m}\right) \overline{r^2}$

4-17-72 MON)

TOTAL ORBITAL ANGULAR MOMENTUM

$|\vec{L}| = \sqrt{L(L+1)}\,\hbar$, L = ORBITAL ANGULAR MOM. QUANTUM NUMBER = INTEGER

$|\vec{S}| = \sqrt{S(S+1)}\,\hbar$, S = TOTAL SPIN ANGULAR MOM. QUANTUM NUMBER = INTEGER/2

$|\vec{J}| = \sqrt{J(J+1)}\,\hbar \Rightarrow J$ = TOTAL TOTAL ANGULAR QUANTUM ANG. MOM. = INTEGER/2

$|\vec{J}| \neq 0$ IF NUMBER OF ELECTRONS IF HAVE UNFILLED INNER SHELL

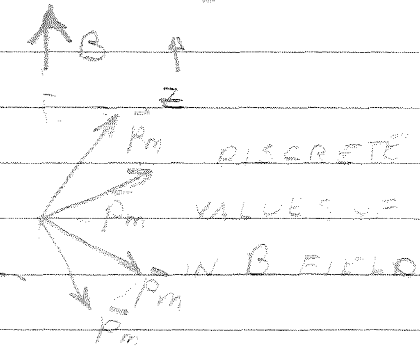
TOTAL MAGNETIC MOMENT

$$\vec{p}_m = -g_J \frac{e}{2m} \vec{J} \qquad g_J = 1 + \frac{J(J+1) - L(L+1) + S(S+1)}{2J(J+1)}$$

APPLY MAGNETIC FIELD TO ATOM HAVING MAGNETIC MOMENT

J_z = Z COMPONENT OF $J \Rightarrow J_z = m_J \hbar$

$\Rightarrow m_J = J, J-1, \ldots\ldots, -J$

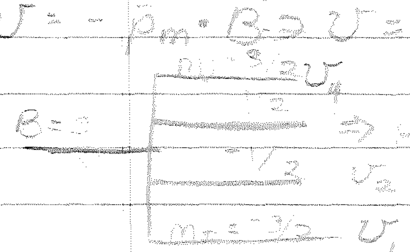


LET $J = 3/2$

$\Rightarrow |\vec{J}| = \sqrt{\frac{15}{4}}\,\hbar$

$m_J = \frac{3}{2}, \frac{1}{2}, -\frac{1}{2}, -\frac{3}{2} \Rightarrow J_z = \frac{3}{2}\hbar, \frac{1}{2}\hbar, \ldots$

NOW $U = -\vec{p}_m \cdot \vec{B} \Rightarrow U$ = ENERGY



AND $(p_m)_z = -g_J \left(\frac{e}{2m}\right) J_z$

$= -g_J \left(\frac{e}{2m}\right) m_J \hbar$

$\Rightarrow U_1 = -(p_m)_z B$

$= g_J \left(\frac{e}{2m}\right)\left(-\frac{3}{2}\right) \hbar B$

$= -\frac{3}{2} g_J \left(\frac{e\hbar}{2m}\right) B$

$= -\frac{3}{2} g_J \beta B \Rightarrow \beta$ = BOHR MAGNETON

$U_2 = -\frac{1}{2} g_J \beta B$

ETC.

PARAMAGNETISM

$$\frac{\int U F(\ ) }{\int F(\ )}$$

$$\bar{U} = \sum U e^{-U/kT} \Big/ \sum e^{-U/kT}$$

$$= \frac{\sum_J m_J g_J \beta B e^{-m_J g_J \beta B/kT}}{\sum_J e^{-m_J g_J \beta B/kT}}$$

$$\bar{U} = -(\bar{p}_m)_z B$$

$$(\bar{p}_m)_z = \sum_J -m g_J \beta e^{-m g_J \beta B/kT} \Big/ \sum_J e^{-m_J g_J \beta B/kT}$$

YIELDING (AFTER INFINATE CRANK)

$$(\bar{p}_m)_z = g_J \beta J \left\{ \left(\frac{2J+1}{2J}\right) \coth\left[\frac{(2J+1)x}{2J}\right] - \frac{1}{2J} \coth\left(\frac{x}{2J}\right) \right\}$$

$$\ni x = g_J \beta J B / kT$$

FOR N ATOMS PER UNIT VOLUME

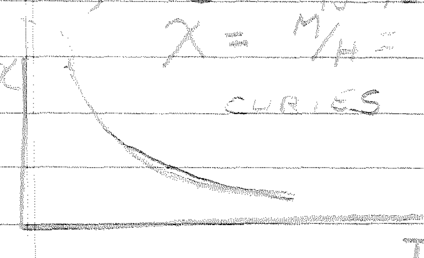
$$\bar{M} = N(\bar{p}_m)_z$$

$$\chi_p = M/H$$

NORMAL T AND B (NOT VERY LOW T OR VERY HIGH B)

$$M = C/T \quad ; \quad C = N g_J^2 \beta J(J+1) B/3k$$

$$\chi = M/H = C/T \quad \text{(SUSCEPTIBILITY)}$$



CURIES LAW

GO TO TUES, Pg 48

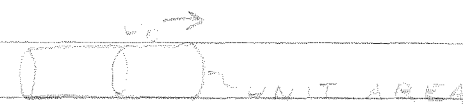
4-12-72 (WED)

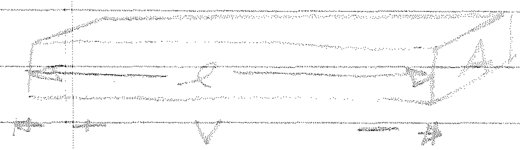
FREE ELECTRON THEORY (METALS) - DRUDE 1900

DRIFT VELOCITY v_D

MOBILITY $\mu = v_D/E \ni E =$ ELECTRIC FIELD

$$|\vec{J}| = I/A = |ne\,\vec{v}_D|$$





$$V = Ri = \frac{\rho \ell}{A} i$$

$$E = \frac{V}{\ell} = \rho i/A = \rho J$$

OR $\vec{E} = \rho \vec{J}$ (ANALAGOUS TO $V = IR$)

ρ = RESISTIVITY $\ni \rho = 1/\sigma \ni \sigma$ = CONDUCTIVITY

$$\Rightarrow \sigma = J/E$$

$$= nev_D/E \quad \ni n = \text{NUMBER OF FREE ELECTR.}$$

$$= ne\mu$$

OIL DROP IN AIR:

$$\Sigma F = eE - \binom{\text{PROP.}}{\text{CONST}} v_D = m\frac{dv_D}{dt}$$

$$\therefore eE - \left(\frac{m}{\tau}\right) v_D = m\frac{dv_D}{dt} \ni \tau = \text{SOME TIME CONSTANT}$$

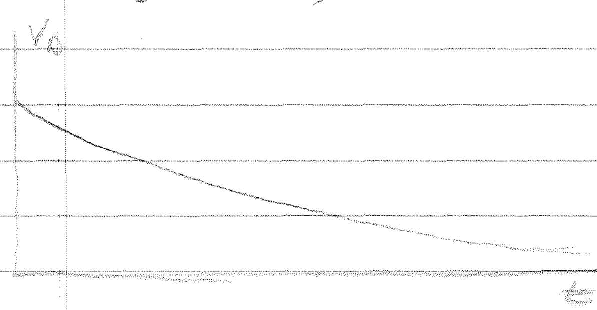
SUPPOSE E HAS BEEN ON $\rightarrow v_D(0)$

TURN OFF.

$$\Rightarrow m\frac{dv_D}{dt} + \frac{m}{\tau} v_D = 0$$

$$\frac{dv_D}{dt} = -\frac{1}{\tau} v_D$$

$$\therefore v_D = v_D(0)\, e^{-t/\tau}$$



τ IS TIME FOR v_D TO DROP TO $1/e$ OF ITS ORIGINAL VALUE $\Rightarrow \frac{1}{e}$ OF THE ELECTRONS HAVEN'T COLLIDED AT END OF τ SECONDS

FIELD ON

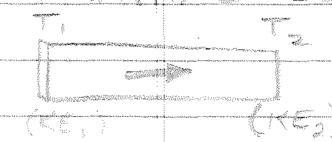
$$eE - \frac{m}{\tau} V_0 = m\frac{dV_0}{dt} = 0$$

$$\rightarrow eE = \frac{M}{\tau} V_0$$

$$\therefore \frac{V_0}{E} = e\tau/m = \mu \Rightarrow \text{(MOBILITITY)}$$

$$\text{AND } \sigma = ne^2\tau/m$$

FOR THERMAL CONDUCTIVITY



$$K = \frac{\pi^2}{3} k^2 T n \frac{\tau}{m} = \text{THERMAL CONDUCTIVITY}$$

k → BOLTZMAN'S CONSTANT

$$L = \frac{K}{\sigma T} = \left(\frac{\pi^2}{3}\right)\left(\frac{k}{e}\right)^2 = \text{LORENZ NUMBER}$$

$$= 2.45 \times 10^{-8} \text{ WATT OHM/DEG}^2$$

SPECIFIC HEAT @ HIGH TEMPERATURES:

$$C_v = 3R \qquad (U = 3RT)$$

FOR FREE e^- CLASSICS SAYS

$$C_v = 3R + \frac{3}{2}R \quad \text{(3 NEW DEGREES OF FREEDOM)}$$

e^- K.E.

NOT SO

$C_v \cong 3R \Rightarrow$ SOMETHING IS INHIBITING ABSORBSION OF ENERGY BY FREE e^-

PARAMAGNETISM OF FREE ELECTRONS

ALIGNMENT OF SPIN MAGNETIC MOMENTS WITH MAGNETIC FIELD.

→ χ MUCH LARGER

EXPERIMENTAL: χ ONLY SLIGHTLY INCREASED BY ALIGNMENT OF FREE ELECTRON MAGNETIC MOMENTS (SOMETHING INHIBITING MOMENT ALIGNMENTS)

GO TO FRI, pg 53

4-24-72 (MON)

FREE ELECTRON THEORY

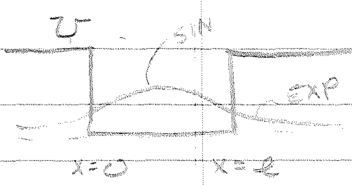
METAL CUBE, EDGE L,

IF ELECTRONS CANNOT BE EMITTED (ie $U=\infty$ OUTSIDE), THE ALLOWED ELECTRON ENERGIES (FROM SCHROEDINGER EQUATION ARE:

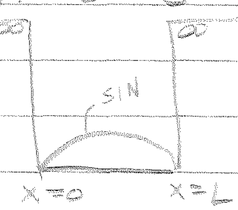
$$E_n = \frac{\hbar^2 \pi^2}{2mL^2}(n_x^2 + n_y^2 + n_z^2)$$

n_x, n_y, n_z = INTEGERS ≥ 1

IF $U<\infty$



IF $U=0$



IF $U \neq \infty$, $L_{EFF} > L$

AGAIN

$$E_n = \frac{\hbar^2 \pi^2}{2mL^2}(n_x^2 + n_y^2 + n_z^2)$$

1) CAN'T DISTINGUISH ELECTRONS (PARTICLES ARE INDISTINGUISHABLE FROM EACH OTHER)

2) EXCLUSION PRINCIPLE - NO TWO PARTICLES ARE IN THE SAME STATE

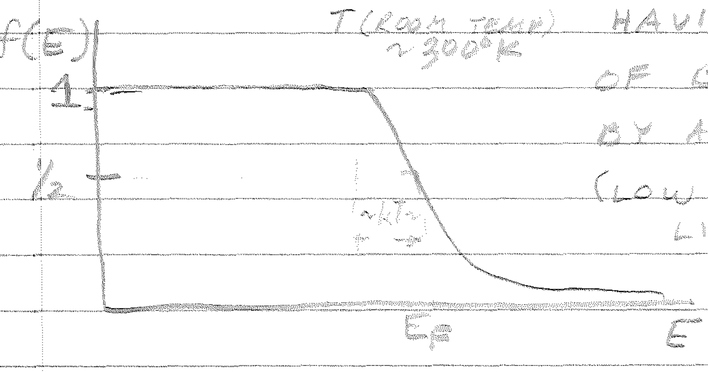
$n_x, n_y, n_z, m_s \longrightarrow$ STATE OF ELECTRONS

YIELDS FERMI-DIRAC STATISTICS (TAKES PLACE OF BOLTZMAN STATISTICS)

PROBABILITY THAT THE STATE OF ENERGY E_i IS "OCCUPIED" BY AN ELECTRON

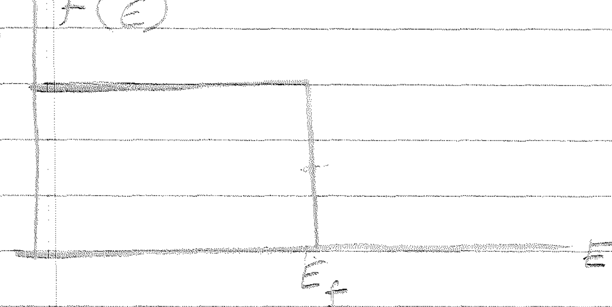
(FERMI FUNCTION: $f(E_i) = \left(e^{(E_i - E_F)/kT} + 1\right)^{-1}$

$\Rightarrow E_F$ = FERMI FUNCTION = ENERGY OF STATE HAVING 50% CHANCE OF BEING OCCUPIED BY AN ELECTRON (LOW ENERGIES MORE LIKELY TO BE OCCUPIED)

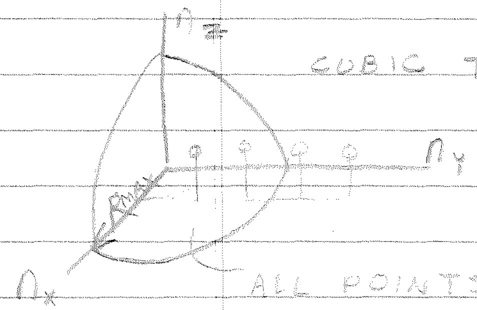


$E_i >> kT$

@ $T = 0°K$



FINDING E_f



CUBIC TYPE LATTICE, EACH POINT REPRESENTS TWO STATES

ALL POINTS (STATES) INSIDE R_{MAX} ARE OCCUPIED @ $T = 0°K$

$$R_{MAX} = (n_x^2 + n_y^2 + n_z^2)^{1/2}_{MAX}$$

$$R_{MAX} = \frac{L\sqrt{2mE_{F_0}}}{\hbar\pi} \quad \text{OR} \quad R_{MAX}^2 = \frac{2mL^2E_{F_0}}{\hbar^2\pi^2}$$

NUMBER OF OCCUPIED STATES HAVING ENERGY $\leq E_{F_0} = E_F$ (SAME AS TWICE SPHERE SECTION VOLUME)

$$= 2\left(\frac{1}{8}\left\{\frac{4}{3}\pi R_{MAX}^3\right\}\right)$$

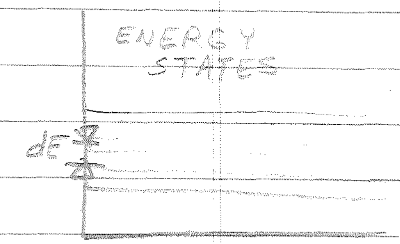
$$= \frac{\pi}{3}\left(2mL^2E_{F_0}/\hbar\pi^2\right)^{3/2}$$

FOR N FREE ELECTRONS, $N = \frac{\pi}{3}\left(\frac{2mL^2E_{F_0}}{\hbar\pi^2}\right)^2$

$$\Rightarrow E_{F_0} = \frac{\hbar^2}{2m}\left(\frac{3\pi^2 N}{L^3}\right)^{3/2}$$

$$= \frac{\hbar^2}{2m}\left(3\pi^2 n\right)^{3/2} \quad \ni n = \text{FREE ELECTRON DENSITY}$$

$\sim$ 1 TO 10 eVOLTS



DEFINE $g(E)dE$ = NUMBER OF STATES WITH ENERGY TWIXT E AND $E+dE$

AND $N(E)dE$ = NUMBER OF ELECTRONS HAVING ENERGY TWIXT E AND $E+dE$

PROB

$\Rightarrow f(E)g(E)dE = N(E)dE$ (FOR ANY T)

@ $T = 0°K$

$f(E) = 1$ UP TO $E = E_{f0}$

$= 0$, ABOVE $E = E_{f0}$

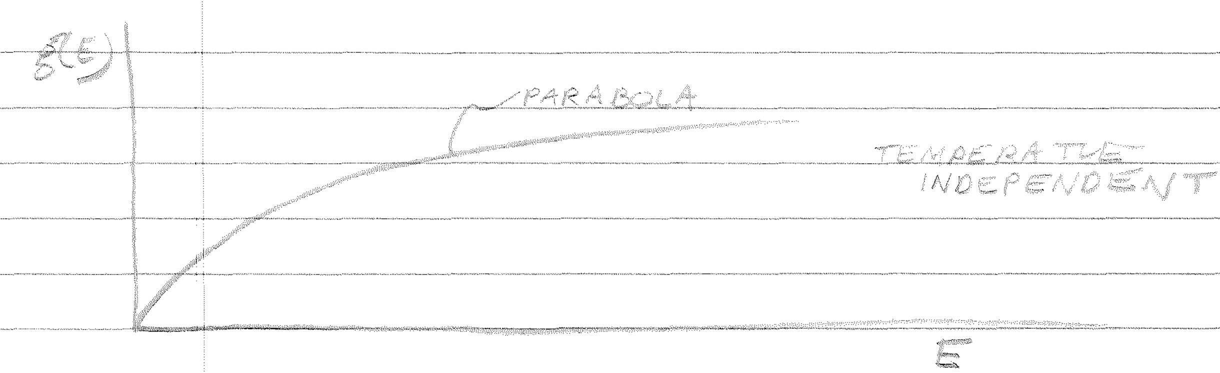
$$N = \int_0^{E_{f0}} N(E)dE = \int_0^{E_{f0}} g(E)dE$$

NOW $N = \frac{L^3}{3\pi^2}\left(\frac{2mE_{f0}}{\hbar^2}\right)^{3/2}$

HENCE

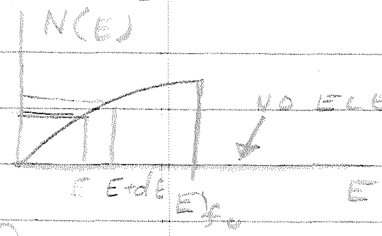
$$\frac{L^3}{3\pi^2}\left(\frac{2mE_{f0}}{\hbar^2}\right)^{3/2} = \int_0^{E_{f0}} g(E)dE$$

$$g(E) = \frac{L^3}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)\sqrt{E} = C\sqrt{E}$$

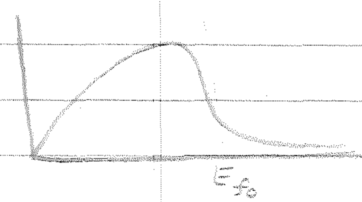


ELECTRON ENERGY DISTRIBUTION

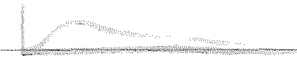
@ $T = 0^\circ$



@ $T > 0^\circ$



FOR REAL HIGH TEMP, A BOLTZMAN DISTRIBUTION IS APPROACHED:



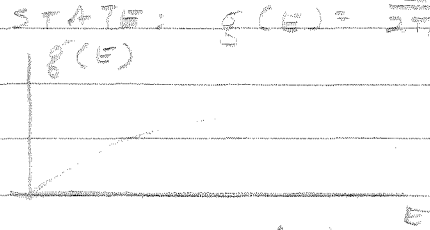
4-25-72 (TUES) TEST FRI

FREE ELECTRON MODEL

$$E = (\hbar^2 \pi^2 / 2mL^2)(n_x^2 + n_y^2 + n_z^2)$$

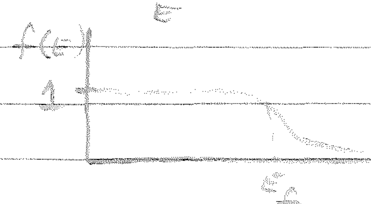
NO MORE THAN 1 ELECTRON PER STATE n_x, n_y, n_z, m_s

DENSITY OF STATE: $g(E) = \frac{L^3}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} E^{1/2} = CE^{1/2}$

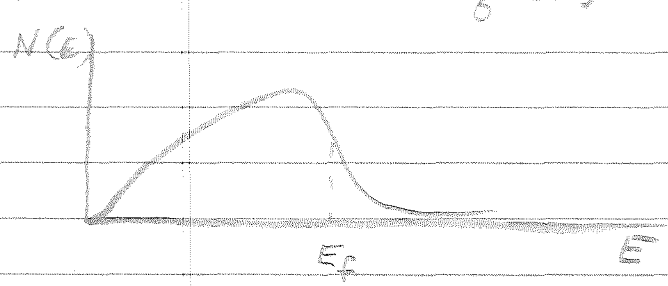


$g(E)dE$ = NUMBER OF STATES HAVING ENERGIES 'TWIXT E AND $E + dE$

$$f(E) = \frac{1}{e^{(E-E_F)/kT} + 1}$$



SUPERPOSING $f(E)$ ON $g(E)$



$T = 0°K \Rightarrow \quad f(E) = 1 \qquad 0 < E < E_f$

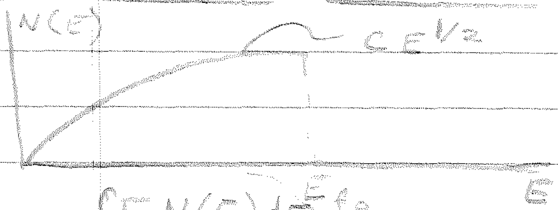
$\qquad\qquad\qquad\quad = 0 \qquad E > E_f$

$$E_{f0} = \frac{\hbar^2}{2m}\left(3\pi^2 n\right)^{2/3}$$

SMALL C_v FOR ELECTRONS DUE TO EXCLUSION PRINCIPLE

AVERAGE ELECTRON ENERGY

1) $T = 0°K$



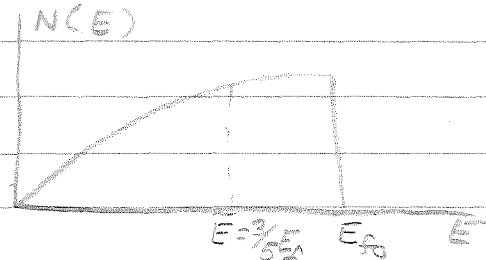
$$\bar{E}(0) = \frac{\int E\,N(E)\,dE}{N} \qquad N = \int_0^\infty N(E)\,dE$$

$$= \int_0^{E_{f0}} C E^{\frac{1}{2}}\,dE = \frac{2}{3} C E_f^{3/2}$$

$$\text{AND} \quad \int_0^\infty E\,N(E)\,dE = \int_0^{E_f} C E^{3/2}\,dE$$

$$= \frac{2}{5} C E_{f0}^{5/2}$$

$$\Rightarrow \bar{E}(0) = \frac{3}{5} E_{f0}$$

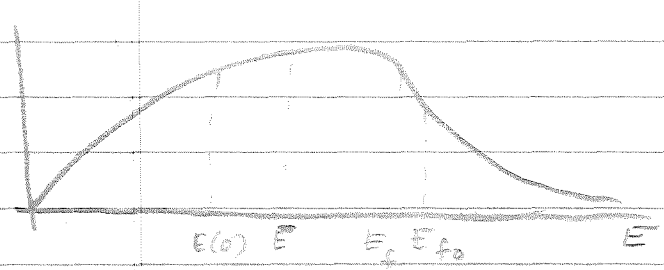


2) $T > 0°K \qquad N = \frac{2}{3} C E_{f0}^{3/2}$ (NUMBER OF e DON'T CHANGE) (FROM ABOVE)

$$\bar{E} = \frac{\int_0^\infty E\,N(E)\,dE}{N} = \frac{\int_0^\infty \frac{C E^{3/2}\,dE}{e^{(E-E_f)/kT}+1}}{N} \qquad f(E)\,C E^{1/2} E\,dE$$

$$\Rightarrow \bar{E} = \bar{E}(0)\left[1 + \frac{5\pi^2}{12}\left(\frac{kT}{E_{f0}}\right)^2\right]$$

$\bar{E}$ INCREASES A LITTLE WITH T, AND E_f DECREASES SLIGHTLY



SPECIFIC HEAT

TOTAL ENERGY IN ELECTRONS:

$$U = N\bar{E} = NE(0)\left[1 + \frac{5\pi^2}{12}\left(\frac{kT}{E_{f0}}\right)^2\right]$$

$$\Rightarrow C_v = \frac{dU}{dT}\Big|_v = NE(0)\frac{5\pi^2 k^2 T}{6E_{f0}^2}$$

NOW $E(0) = \frac{3}{5}E_{F0}$

$$\Rightarrow (C_v)_{el} = \frac{N\pi^2 k^2 T}{2E_{f0}}$$

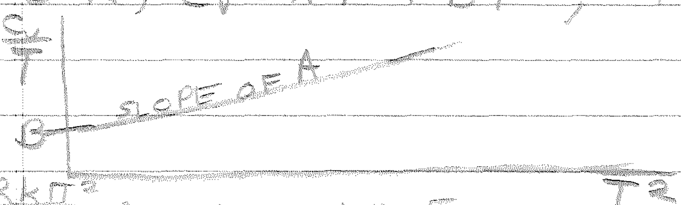
SUPPOSE, 1 MOLE: N_0 ATOMS WITH 1 el/ATOM FREE.

$$\Rightarrow (C_v)_{el} = \frac{(N_0 k)kT\pi^2}{2E_{f0}}$$

$$= RkT\pi^2/2E_{f0} << \frac{3}{2}R$$

$$\frac{\delta U}{\delta T}\Big]_v = C_v = (C_v)_{VIB} + (C_v)_{ELEC}$$

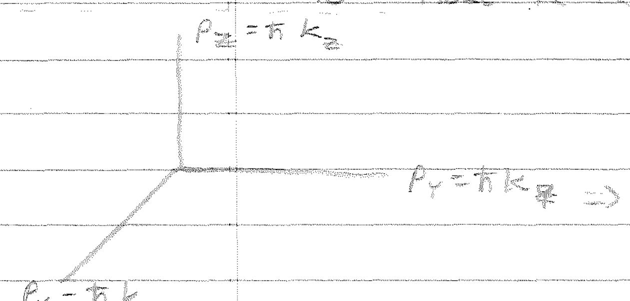
AS $T \to 0°K$; $C_v = AT^3 + BT$; $T^3 << T$



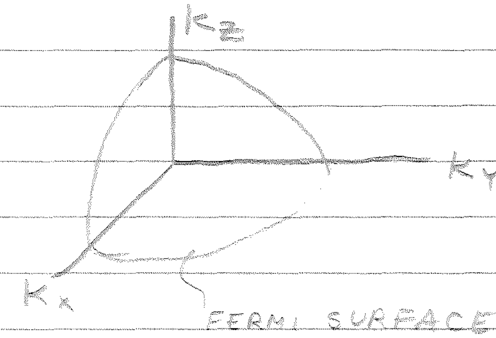
$B = \frac{Rk\pi^2}{2E_{f0}}$; MAY FIND E_{f0}

IN COPPER: $B = \frac{1.78 \text{ CAL}}{\text{MOLE } °K °K}$ (EXPERIMENTAL)

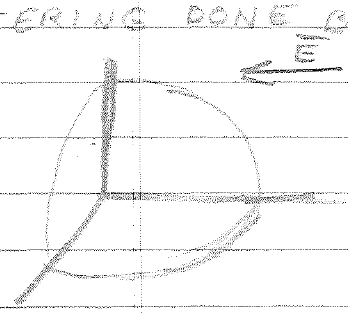
$B = \frac{1.24 \text{ CAL}}{\text{MOLE } °K °K}$ (THEORY)



$p = \hbar k$ = ELEC MOMENTUM



SCATTERING DONE BY e NEAR FERMI SURFACE

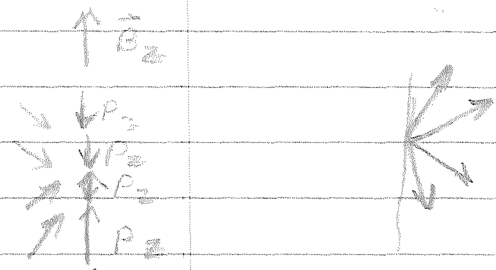


$\bar{E}$ WILL SHIFT FERMI SURFACE

SHIFT = $m_1 v_0/\hbar$

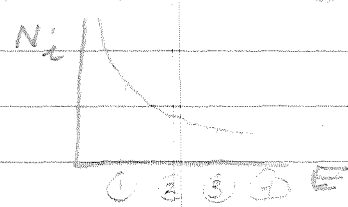
4-18-72 (TUES)

PARAMAGNETISM - MAGNETIC MOMENTS AID APPLIED FIELD



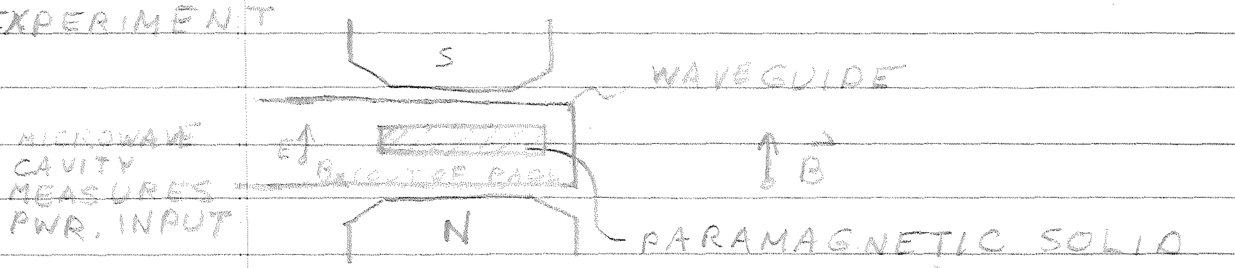
BOLTZMAN DISTRIBUTION; $N \alpha\ ^{-U/kT}$

THE HIGHEST NUMBER OF PARTICLES WILL BE IN STATE ① WHERE P_z IS LARGEST IN THE DIRECTION OF B_z



SPACING 'TWIXT ENERY LEVELS $\Delta U = g_J \beta B \ni \beta = \frac{e\hbar}{2m}$

EXPERIMENT



MICROWAVES OF FREQUENCY f

PHOTONS OF ENERGY $E = hf$

IF $\vec{B}$ IS INCREASED GRADUALLY → INCREASING SPACING TWIXT ENERGY LEVELS

WHEN $\vec{B}$ IS $\ni$ $g_J \beta B = hf$, THERE WILL BE RESONANT ABSORBTION

MEASURE THE VALUE OF $\vec{B}$ FOR WHICH YOU GET A SUDDEN INCREASE IN PWR. INPUT

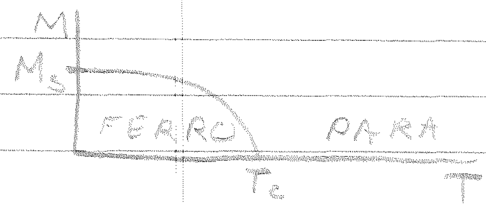
CAN NOW COMPUTE g_J FOR THE SOLID

THIS EXPERIMENT IS ALSO USED TO DETERMINE INTERNAL FIELDS, AND IS CALLED ELECTRON PARAMAGNETIC RESONANCE (EPR)

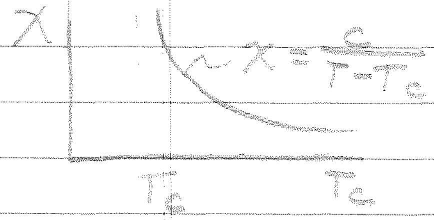
FERROMAGNETISM

SPONTANEOUS MAGNETISM WITH NO APPLIED FIELD

M VERY LARGE COMPARED WITH PARAMAGNETIC

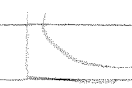


SUSCEPTIBILITY OF FERROMAGNETIC



CURIE-WEISS

RECALL FOR PARAMAGNETIC: $\chi = C/T$



WEISS

COOPERATIVE EFFECT - MAGNETIC MOMENTS TEND TO LINE UP NEIGHBORING $\vec{p}_m$ IN SAME DIRECTION.

AT THE POSITION OF THE ATOM:

$H_{eff} = H + \lambda M$ ← DUE TO ALIGNMENT

ABOVE THE CRITICAL T_c IT'S A PARAMAGNETIC MATERIAL

$$\Rightarrow \chi = M/H_{eff} = C/T$$

(NEIGHBORING MOMENTS BEGIN TO HAVE LESS EFFECT ON EACH OTHER PAST T_c)

$$\frac{M}{H + \lambda M} = \frac{C}{T} \qquad \chi = \frac{M}{H} = C/T - c\lambda$$

$$M = \frac{C}{T}(H + \lambda M) \qquad \chi = C/T - T_c$$

$$M = CH/T - c\lambda$$

WHAT CAUSES THESE MAGNETIC MOMENTS TO ALIGN EACH OTHER?

"EXCHANGE" FORCE CAUSES NEIGHBORING SPIN MAGNETIC MOMENTS OF OUTER ELECTRONS IN CERTAIN ATOMS TO BE IN THE SAME DIRECTION

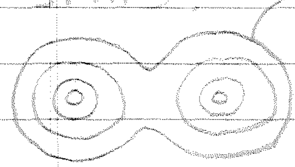
LOOK @ THE HYDROGEN MOLECULE

2 POSSIBILITIES

1) THE ELECTRONS HAVE THE SAME SPIN, EXCLUSION PRINCIPLE TENDS TO FORCE APART

2) THE TWO ELECTRONS HAVE OPPOSITE SPIN

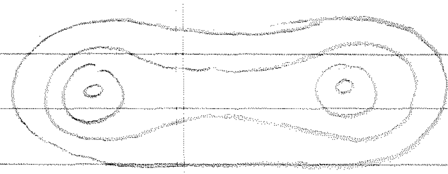
PARALLEL SPINS:



CONSTANT PROBABILITY LINES OF ELECTRON LOCATION

LOW PROBABILITY OF FINDING A "SHARED" ELECTRON

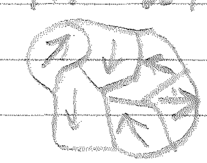
ANTI PARALLEL SPINS:



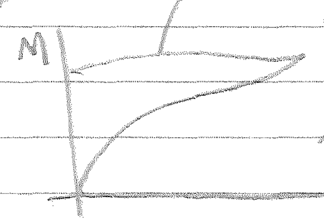
LOWEST COULOMB POTENTIAL ENERGY

IN FERROMAGNETIC MATERIALS THE PARALLEL SPIN CONFIGURATION HAS LOWEST ENERGY. PARALLEL SPINS IN ADJACENT ATOMS (Fe, Ni, Co)

DOMAINS IN WHICH M IS IN ONE DIRECTION



HYSTERESIS



BOUNDRIES WON'T RE-ALIGN EXACTLY AS BEFORE THE FIELD IS APPLIED. (LEFT WITH A NET MAGNETIZATION)

GO TO WED, PG 40

4-27-72 (WED)

PARAMAGNETISM OF FREE ELECTRON

$|\vec{p}_m| = g\left(\frac{e}{2m}\right)\vec{S}$

$\uparrow \vec{B}_z$

PAR.

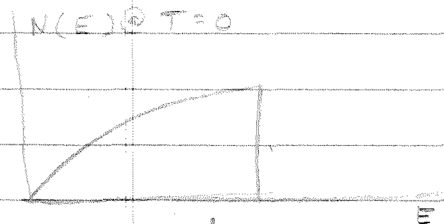
$+\frac{e\hbar}{2m}$ $\quad (p_m)_z = g\left(\frac{e}{2m}\right)S_z \Rightarrow S_z = \pm\frac{1}{2}\hbar$ AND $g \simeq 2$

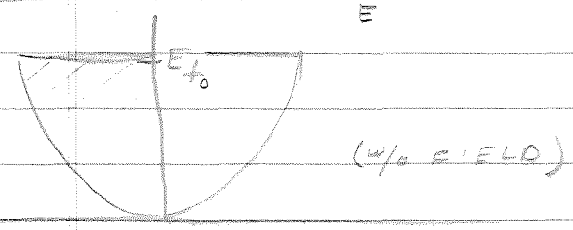
ANTIPAR. $\Rightarrow (p_m)_z = \pm\left(\frac{e\hbar}{2m}\right)$

$U = \vec{p}_m \cdot \vec{B} = -(p_m)_z B$ (PAR. HAVE LOWEST ENERGY)

- - - - - - - - - - -

$n_x, n_y, n_z, m_s = \pm\frac{1}{2}$; $m_s\hbar = S_z$

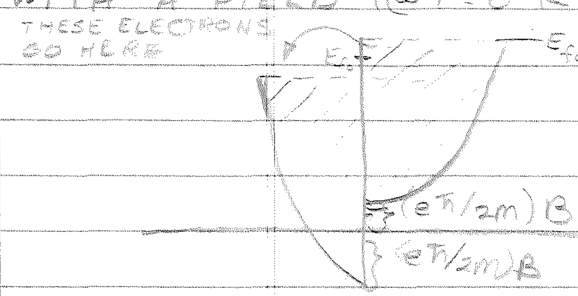




N(E) PARALELL $\qquad$ N(E) ANTIPARALLEL

$\ni N(E) =$ NUMBER OF ELECTRONS WITH ENERGY 'TWIXT E & E+dE

WITH A FIELD (@T=0°K)



THE NUMBER OF SPIN $\vec{p}_m$ THAT CHANGED FROM ANTIPARALLEL TO PARALLEL $= \frac{1}{2}N(E_{f_0})\Delta E$

$\Delta E = \left(\frac{e\hbar}{2m}\right)B$

EXCESS PARALLEL PER ELECTRON $= N(E_{F_0})\,dE$

$$N(E)\,dE = CE^{1/2}\,dE$$
$$= \frac{1}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} E_{F_0}^{1/2}\,dE$$

$$\Rightarrow E\text{-}P/E = \frac{1}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} E_{F_0}^{1/2}\,(p_m)_z\,B$$

M = MAGNETIC MOMENT PER UNIT VOLUME (M)

$$M = \left[\frac{1}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} E_{F_0}^{1/2}(p_m)_z B\right](p_m)_z$$

ASSUMING N/UNIT VOLUME

χ = SUSCEPTIBILITY = M/H AND $B = \mu H \approx \mu_0 H$

$$\Rightarrow \chi = \frac{M}{H} = \left[\frac{\mu}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} E_{F_0}^{1/2}(p_m)_z^2\right] \quad \mu \approx \mu_0$$
$$= \frac{M}{H} = \left[\mu/2\pi^2\,(2m/\hbar^2)^{3/2}\,E_{F_0}^{3/2}\,(p_m)_z^2 \big/ E_{F_0}\right]$$
$$= 3n\mu\,(p_m)_z^2 / 2E_{F_0}$$

TEST REVIEW

DISCRIPTION AND ALGEBRAIC DERIVATION

A) ATOMIC DIAMAGNETISM

B) ATOMIC FERROMAGNETISM

1) (CURIE LAW FOR NORMAL B AND T)

2) PARAMAGNETIC RESONANCE

C) FERROMAGNETISM

1) WEISS INTERNAL FIELD

2) CURIE WEISS LAW IN PARAMAGNETIC REGION

3) EXCHANGE FORCES

4) SPONTANEOUS $\bar{M}$

5) DOMAINS

6) HYSTERISIS

D) FREE ELECTRON THEORY

1) MODEL

2) CONDUCTIVITY $\sigma(\tau, m, e, n)$

3) IN QUANTUM MECHANICS

a) DETERMINATION OF ELECTRON ENERGY

– DEFINED ELECTRON STATE – EXCLUSION PRINCIPLE, FERMI ENERGY, FERMI SURFACE IN K (MOMENTUM SPACE)

b) DETERMINATION OF FERMI E. @ T = 0°K as $f(N_e/V)$

3) DETERMINATION OF THE DENSITY OF STATES

$\sigma(E) = CE^{1/2}$

4) AVERAGE ELECTRON ENERGY @ $T = 0°K$, DEPENDENCE ON T, AND ELECTRONIC SPECIFIC HT.

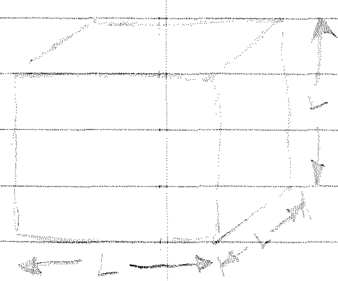
5) FREE ELECTRON PARAMAGNETISM

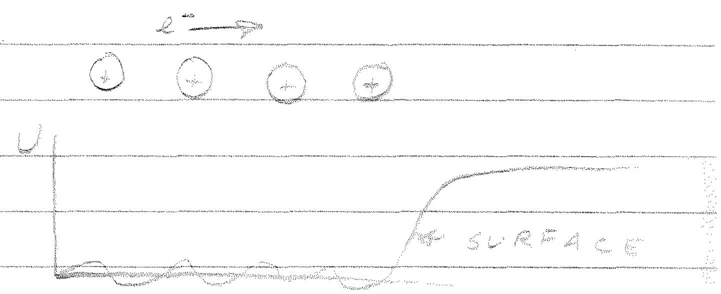
- DETERMINATION OF SUSCEPTIBILITY @ $T = 0°K$

GO TO MON

FRI (4-21-72)

FREE ELECTRONS IN A METAL





ELECTRONS CONFINED TO BOX

$U = 0$ INSIDE; $U = \infty$ OUTSIDE

$-\frac{\hbar^2}{2m}\nabla^2\psi + U\psi = E\psi$; IF $|\psi|^2$ IS TIME INDEPENDENT

$\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2} + \frac{2m}{\hbar^2}E\psi = 0$

$U = 0$ @ EDGES AND ~~OUTSIDE~~ INSIDE

$\Rightarrow \psi(x,y,z) = C \sin\left(\frac{n_x \pi x}{L}\right)\sin\left(\frac{n_y \pi y}{L}\right)\sin\left(\frac{n_z \pi z}{L}\right)$

$n_x, n_y, n_z \in$ P.I.

$-\frac{n_x^2\pi^2}{L^2}\psi - \frac{n_y^2\pi^2}{L^2}\psi - \frac{n_z^2\pi^2}{L^2}\psi = -\frac{2mE}{\hbar^2}\psi$

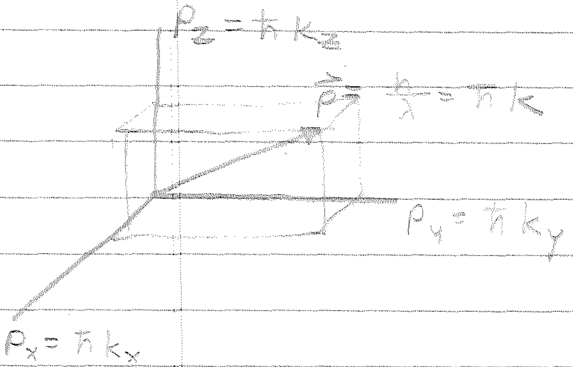
$E = \frac{\hbar^2\pi^2}{2mL^2}(n_x^2 + n_y^2 + n_z^2) \Rightarrow$ ONLY ALLOWED ENERGIES

THE STATE OF MOTION OF THE ELECTRONS DETERMINED BY n_z, n_y, AND n_x

$$E = \frac{p^2}{2m} = \frac{p_x^2 + p_y^2 + p_z^2}{2m}$$

$$= \frac{\hbar^2\pi^2}{2mL^2}(n_x^2 + n_y^2 + n_z^2)$$

$$p_x = \frac{\hbar\pi n_x}{L};\quad p_y = \frac{\hbar\pi n_y}{L};\quad p_z = \frac{\hbar\pi n_z}{L}$$



m_s DETERMINES THE DIRECTION OF THE Z COMPONENT OF THE SPIN ANGULAR MOMENTUM IN PRESENTS OF MAGNETIC FIELD

EXCLUSION PRINCIPLE

NO TWO ELECTRONS IN THE SAME SYSTEM (CUBE) ARE ALLOWED TO HAVE THE SAME 4 QUANTUM NUMBERS HAVE THE SAME QUANTUM NUMBERS (n_x, n_y, n_z, m_s)

→ NO TWO ELECTRONS IN SAME STATE OF MOTION

@ $T = 0°K$, ALL STATES UP TO E_f ARE OCCUPIED BY AN ELECTRON EACH, NO STATES ABOVE E_f ARE OCCUPIED

$$(C_v)_{ELEC} = \frac{dU}{dT}$$

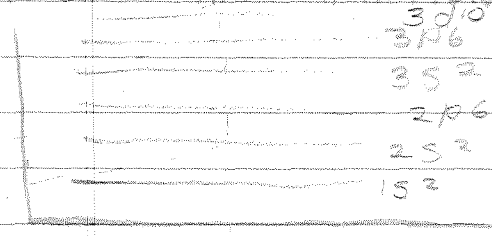
EXCLUSION PRINCIPLE CAUSES C TO BE LOWER THAN USUAL

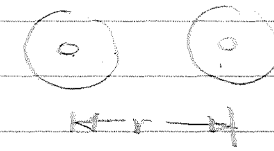
5 - 71 NEW TEST

BAND THEORY

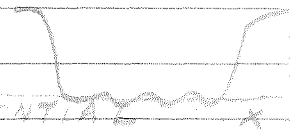
TREAT ALL ELECTONS ALIKE

1) TIGHT BAND APPROXIMATION





2) NEARLY FREE ELECTRON APPROXIMATION



ELECTRONS IN A PERIODICALLY CHANGING POTENTIAL

a) TUNNELING

b) NEARLY FREE ELECTRON

PERFECTLY FREE ELECTRON

$$\nabla^2\psi + \frac{2m}{\hbar^2}E\psi = 0 \quad ; \quad U = 0 \qquad \left(E = \frac{p^2}{2m}\right)$$

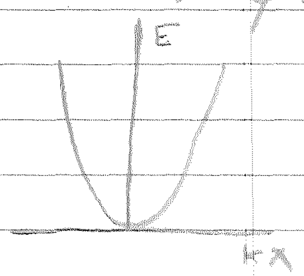
$$\nabla^2\psi = \frac{-2mE}{\hbar^2}\psi$$

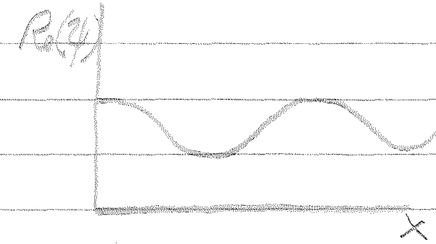
$$k = \frac{p}{\hbar} = \sqrt{2mE}/\hbar \Rightarrow E = \frac{\hbar^2 k^2}{2m}$$

$$\nabla^2\psi = -k^2 x$$

IN ONE DIMENSION: $\nabla^2\psi = k^2 x$

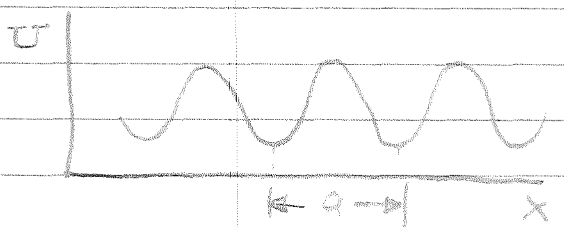
$$\Rightarrow \psi = Ce^{ikx}$$





$k = \frac{p}{\hbar} > 0$ FOR MOTION TO THE RIGHT

$k < 0$ FOR MOTION TO THE LEFT



$U(x+a) = U(x)$

$\nabla^2\psi + \frac{2m}{\hbar^2}(E-U)\psi = 0$

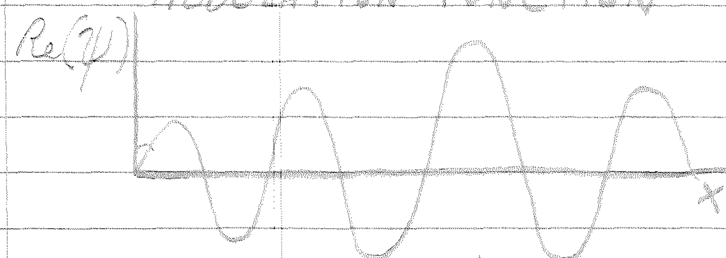
FOR THE X DIRECTION

$\frac{\delta^2\psi}{\delta x^2} + \frac{2m}{\hbar^2}\left[E - U(x)\right]\psi = 0$

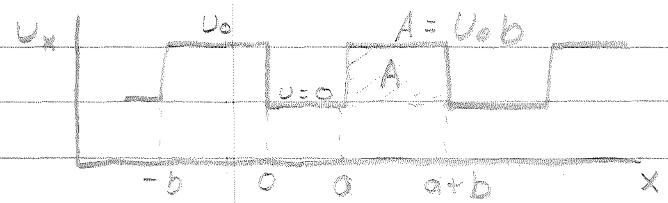
$\psi = U_k(x)e^{ikx}$ (BLOCH FUNCTIONS)

$U_k(x+a) = U_k(x)$

MODULATION FUNCTION



KRONIG-PENNEY MODEL



$0<x<a$; $\frac{\delta^2\psi}{\delta x^2} + \left(\frac{2m}{\hbar^2}\right)E\psi = 0$

$-b<x<0$; $\frac{\delta^2\psi}{\delta x^2} + \left(\frac{2m}{\hbar^2}\right)E\psi = 0$

$\alpha^2 = 2mE/\hbar^2$; $\beta^2 = 2m(U_0 - E)/\hbar^2$

$\psi = U_k(x)e^{ikx}$

$U_1 = Ae^{i(\alpha-k)x} + Be^{-i(\alpha+k)x}$

$U_2 = Ce^{(\beta-ik)x} + De^{-(\beta+ik)x}$

$U_1(0) = U_2(0)$; $\left(\frac{\delta U_1}{\delta x}\right)\Big|_{x=0} = \left(\frac{\delta U_2}{\delta x}\right)\Big|_{x=0}$

$U_1(a) = U_2(-b)$; $\left(\frac{\delta U_1}{\delta x}\right)\Big|_{x=a} = \left(\frac{d U_2}{d x}\right)\Big|_{x=-b}$

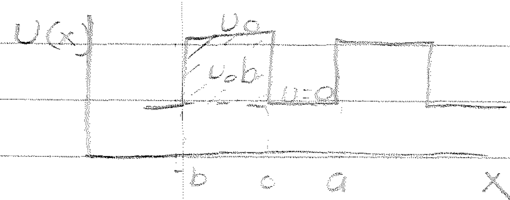
$$\Rightarrow \underbrace{\frac{\beta^2-\alpha^2}{2\alpha\beta}}_{=\frac{mU_0}{\hbar^2\alpha\beta}} \sinh\beta b \sin\alpha a + \cosh\beta b\cos\alpha a = \cos k(a+b)$$

LET $U_0 \to \infty$; $b \to 0$

5-2-72 (TUES)

ELECTRON IN A PERIODIC POTENTIAL

KRONIG-PENNY MODEL



SCHROEDINGER EQUATION GIVES

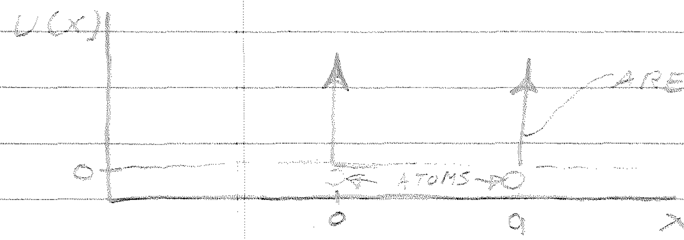
$$\frac{mU_0}{\hbar^2\alpha\beta}\sinh\beta b\sin\alpha a+\cosh\beta b\cos\alpha a=\cos k(a+b)$$

$$\frac{mU_0 b}{\hbar^2\alpha}\frac{\sinh\beta b}{\beta b}\sin\alpha a+\dots$$

$$\alpha=\sqrt{2mE}/\hbar$$

$$\beta=\frac{\sqrt{2m(U_0-E)}}{\hbar}$$

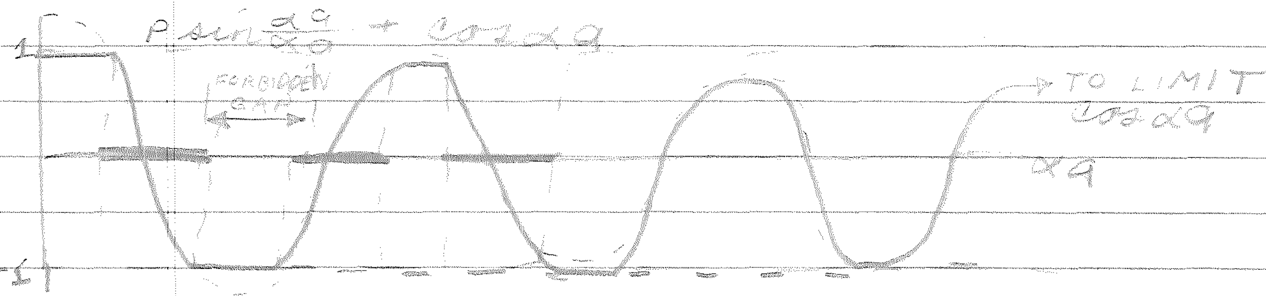
LET $b\to 0$, AND $U_0\to\infty$, $\ni U_0 b=$ CONSTANT



$$\Rightarrow \frac{mU_0 b}{\hbar^2\alpha}\sin\alpha a+\cos\alpha a=\cos ka=\frac{mU_0ba}{\hbar^2}\frac{\sin\alpha a}{\alpha a}+\cos\alpha a$$

$$=P\frac{\sin\alpha a}{\alpha a}+\cos\alpha a=\cos ka$$

$$\Rightarrow P=mU_0ba/\hbar^2$$



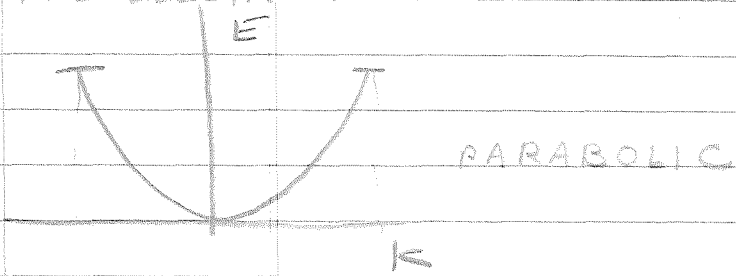
BUT RIGHT SIDE HAS LIMITS OF $-1<$ TO >1

$\Rightarrow$ CERTAIN VALUES OF α ONLY

AS α INCREASES, GAP LENGTHS INCREASES

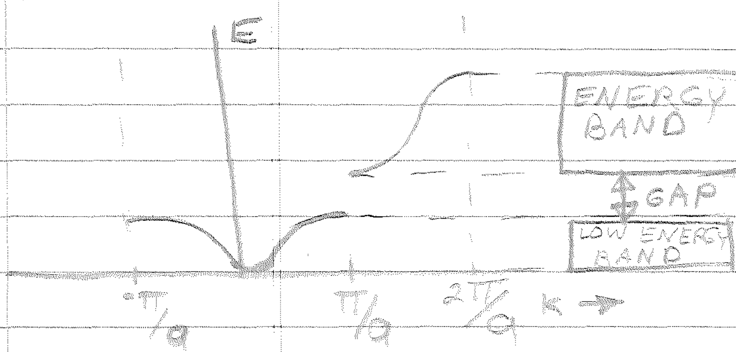
(FORBIDDEN GAPS DECREASE)

FREE ELECTRON



IN A PERIODIC POTENTIAL

$E(K) = E(-K)$



$\ominus$ WAVE @ $k = \pi/a = 2\pi/\lambda \Rightarrow \lambda = 2a$

FIRST ORDER BRAGG'S LAW

$n\lambda = 2\pi \sin\theta$ (DIFFRACTION)

$-\frac{\pi}{a} < k < \frac{\pi}{a} \Rightarrow$ FIRST BRILLOUIN ZONE

$|\pi/a| < k < |\frac{2\pi}{a}| \Rightarrow$ SECOND " "

$p \neq \hbar k$ ANYMORE

$\hbar k$ = CRYSTAL MOMENTUM (ENERGY OF FREE e^-)

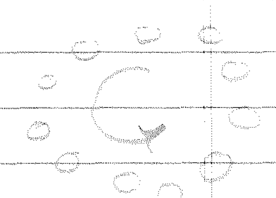
$\hbar k$ IS CONSERVED

NUMBER OF STATES PER BAND

$| \underset{1}{O} \; \underset{2}{O} \; \underset{3}{O} \; O \cdots O O O \underset{N}{O} |$

$x = 0$ $\quad x = L = Na$

BEND IT IN A CIRCLE



$\psi(x) = \psi(x + L)$

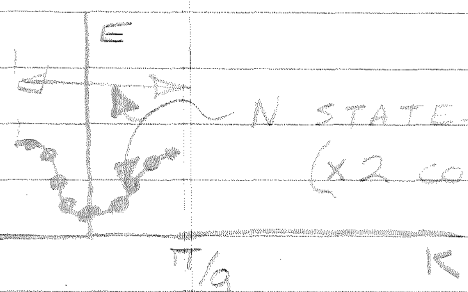
PERIODIC BOUNDRY CONDITIONS

$\psi(x) = \mu_k(x) e^{ikx}$

$\psi(x) = \mu_k(x + Na) e^{ik(x+Na)}$

NOW $\mu_k(x) = \mu_k(x + a) = \mu_k(x + Na)$

$\Rightarrow e^{ikNa} = 1 \Rightarrow kNa = 2\pi n$; $n = \pm 1, \pm 2, \ldots, \pm N/2$



N STATES PER BAND
(X2 CONSIDERING e SPIN)

DENSITY OF STATES

1 STATE PER $\Delta K = \frac{2\pi}{Na}$ @ $X = 0$

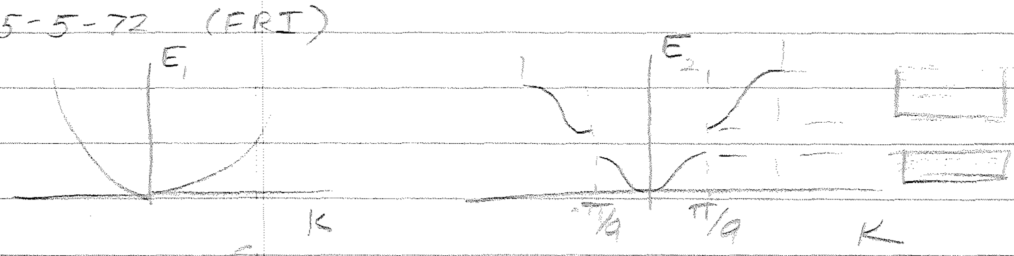
$\frac{N/2}{\pi/a} = \frac{1}{2\pi/Na}$

STATES PER UNIT K

$\frac{dn}{dk} = \frac{1}{\Delta K} = \frac{Na}{2\pi}$

GO TO pg (73) - 5-3-72 (TUES)

5-5-72 (FRI)



$a = {}^{eE}/_{m}$; $\sigma = {}^{ne^2\tau}/_{m}$ FOR E_1

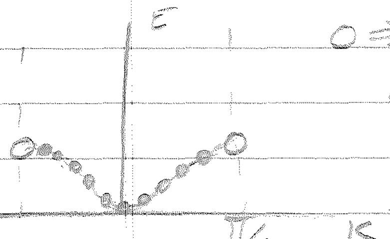
FOR E_2; $a = {}^{eE}/_{m^*} \Rightarrow m^* =$ EFFECTIVE MASS

$\sigma = \frac{ne^2\tau}{m^*}$ $\left(m^* = \hbar^2 \left(\frac{\partial^2 E}{\partial K^2}\right)^{-1} \right.$

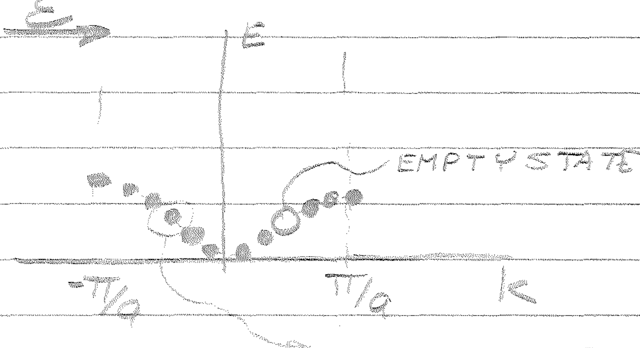
NEARLY FULL CONDUCTION BAND

O ⇒ NOT OCCUPIED (HOLE)

APPLY ℰ FIELD, ACC e'S TO LEFT



$\xrightarrow{\mathcal{E}}$



EMPTY STATE

YIELDS NET ELECTRON

I) QUANTUM MECHANICS REVIEW (DOUBLE ARG)

A) DUAL PROPERTIES OF LIGHT:

MATTER (PHOTON)

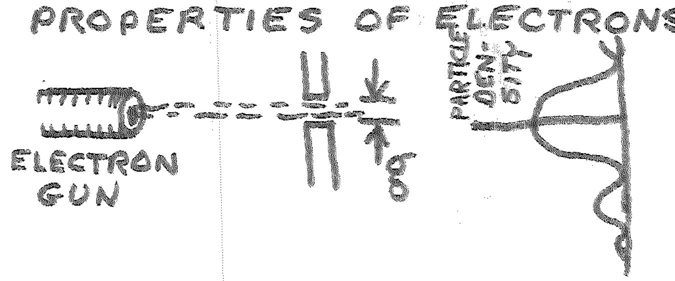
WAVE (ELECTROMAGNETIC)

$E = hf$ (ENERGY IS PROPORTIONAL TO FREQUENCY)

$p = h/\lambda$ (MOMENUM INVERSLY PROPORTIONAL TO WAVELENGTH)

$\bar{p} = \hbar k \ni \vec{k} = 2\pi/\lambda \ni \vec{k}$ IS IN DIRECTION OF THE WAVE ~~FREQ~~ MOTION; $\hbar = h/2\pi$

B) WAVE PROPERTIES OF ELECTRONS:



FROM THIS EXPERIMENT, ONE MAY DETERMINE:

$p = h/\lambda$

AND

$E = p^2/2m + V \ni V =$ POTENTIAL E

DUAL NATURE OF WAVES AND PARTICLES:

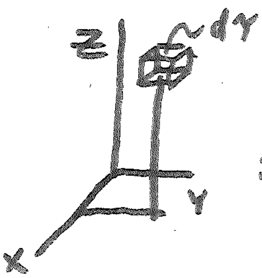
LIGHT: $E = hf$ $\quad p = \hbar \bar{k} = h/\lambda$

MATTER: $E = p^2/2m$ $\quad p = \hbar k = h/\lambda$

C) HEISENBURG'S UNCERTAINTY PRINCIPLE: ONE CANNOT SIMULTANEOUSLY DETERMINE A POSITION CO-ORDINATE AND THE CORRESPONDING MOMENTUM CO-ORDINATE TO ANY GREATER PERCISION THAN:

$$(\Delta p_x)(\Delta x) \geq h$$

THE PROBABILITY OF FINDING A PARTICLE IN THE VOLUME $d\tau$ AT POSITION X, Y, Z:



$P = \int_\tau |\psi|^2 d\tau \ni \psi$ IS THE WAVE FUNCTION, VALUED AT ALL POINTS IN SPACE, MAY BE REAL OR COMPLEX

D) SCHROEDINGER'S EQUATION (CONSERVATION OF E)

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = E\psi \quad \text{(TIME INDEPENDENT)}$$

(EXAMPLE 1) THE VIBRATING ATOM

$V = \frac{1}{2}kx^2$

$$\Rightarrow \frac{\hbar^2}{2m}\frac{\delta^2\psi}{\delta x^2} + \frac{1}{2}kx^2\psi = E\psi$$

SOLUTION YIELDS: $E_n = \frac{2n-1}{2}hf$:

NOTE: NO SOLUTION FOR $E=0 \Rightarrow$ ATOM IS NEVER AT REST!

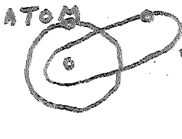
(EXAMPLE 2) ONE ELECTRON ATOM : $V = \frac{1}{4\pi\epsilon_0}\frac{q^2}{r}$

YIELDING

$E_n = -C/n^2 \ni n = 1, 2, 3, 4, 5, \ldots$ (PRINCIPLE QUANTUM #'S)

E) QUANTUM NUMBERS

1) ATOM



ROTATIONAL

$\vec{l} = \vec{r} \times \vec{p}$ (ANGULAR MOMENTUM)

BOTH PATHS HAVE SAME E, BUT DIFFERENT $\vec{l}$

$|\vec{l}| = [l(l+1)]^{1/2}\hbar \ni l = n-1, n-2, \ldots, 0$ (SAME n AS ABOVE)

n: PRINCIPLE QUANTUM NUMBERS

l: AZIMUTHAL QUANTUM NUMBERS

$l = 0 \Rightarrow s$ ELECTRON

$l = 1 \Rightarrow p$ "

$= 2 \Rightarrow d$ "

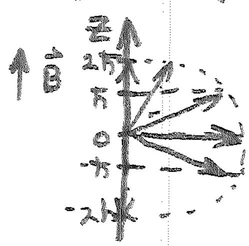
$= 3 \Rightarrow f$ "

2) ELECTRON SPIN ANGULAR MOMENTUM $\vec{s}$

~~$\vec{s} = [s(s+1)]^{1/2}\hbar \ni$~~

$|\vec{s}| = \sqrt{3/4}\,\hbar$

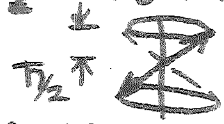
3) IN MAGNETIC FIELD, ONLY CERTAIN DIRECTIONS ARE ALLOWED FOR $\vec{l}$ AND $\vec{s}$



$l_z = m\hbar \ni m = 2, 1, 0, -1, -2$

(SWEEPS A CONE)

$s_z = m_s\hbar \ni m_s = \pm 1/2$



$|\vec{s}| = \sqrt{3/4}\,\hbar$

4) PAULI-EXCLUSION PRINCIPLE (APPLIES TO ODD HALF INTEGRAL SPIN PARTICLES): NO TWO ELECTRONS IN THE SAME QUANTUM-MECHANICAL SYSTEM MAY HAVE IDENTICAL SETS OF QUANTUM NUMBERS (n, l, m, m_s)

H (1 0 0 +1/2) 1s

He (1 0 0 −1/2) $1s^2$

Li (2 0 0 +1/2) $1s^2 2s$

Be (2 0 0 −1/2) $1s^2 2s^2$

~~B~~ ETC.

n: ENERGY

l: ORBITAL ANGULAR MOMENTUM

m = z DIRECTION OF $\vec{l}$

m_s = z COMPONENT OF $\vec{s}$

$s = \pm 1/2$

II) SOLIDS AND FORCES 'TWIXT ATOMS IN 'EM

A) CLASSIFICATIONS OF SOLIDS

1) AMORPHONE SOLIDS: RANDOM ATOMIC ARRANGEMENT (VERY HAIRY TO ANILIZE)

2) CRYSTALLINE SOLIDS: REGULAR ATOM ARRANGEMENT (THESE, WE STUDY)

B) FORCES 'TWIXT ATOMS

1) IONIC FORCES (SUCH AS Na^+Cl^-)

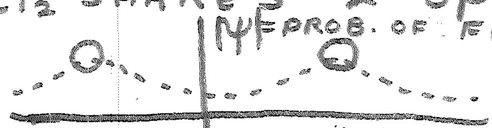
a) COULOMB ATTRACTION OF IONS

b) SUPER STRONG FORCE

① HIGH MELTING POINT

② LOW ELECTRICAL-THERMAL CONDUCTION

2) COVALENT FORCE (SHARED ELECTRONS) (SUCH AS Cl_2) (Cl_2 SHARES 2 3P ELECTRONS)

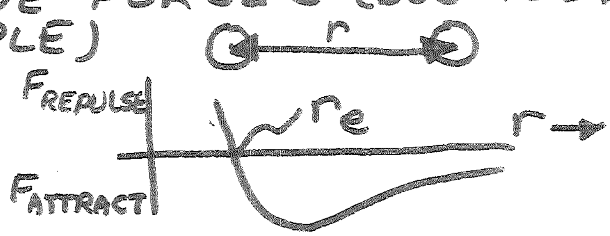


A FAIRLY STRONG FORCE

3) METALLIC BOND-SHARED ELECTRONS 'TWIXT ALL ATOMS OF THE MATERIAL

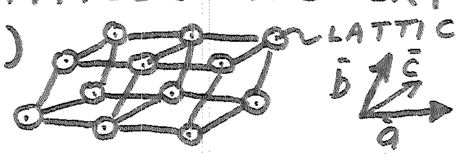
4) VAN-DER-WAALS FORCE (MOLECULAR CRYSTALS) A VERY WEAK DIPOLE ATTRACTIVE FORCE THESE MATERIALS ARE SOLID ONLY AT TEMPERATURES NEAR 0° K

5) REPULSIVE FORCES (DUE TO EXCLUSION PRINCIPLE)



III) LATTICES AND CRYSTAL STRUCTURE

A)



TO GET FROM ONE LATTICE POINT TO ANOTHER:

$\bar{T} = \bar{m}_1\vec{a} + \bar{m}_2\vec{b} + m_3\vec{c}$

$\ni m_1, m_2, m_3$ ARE INTEGERS

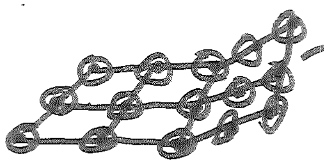
VOLUME OF "UNIT CELL" $= \bar{a} \times \bar{b} \cdot \bar{c}$ (PRIMITIVE UNIT CELL)
↳ PTS. ONLY @ CORNERS

SPACE LATTICE: REGULAR REPEATING ARRANGEMENT OF POINTS SUCH THAT THE ARRANGEMENT OF ATOMS ABOUT EACH POINT IS IDENTICAL

PRIMITIVE UNIT CELL - UNIT CELL HAVING SMALLEST POSSIBLE VOLUME

SINGLE CRYSTAL - LATTICE CONTINUES FROM ONE EDGE OF THE CRYSTAL TO THE OTHER WITH NO BREAKS

POLYCRYSTALINE - BREAKS IN THE LATTICE



~ GRAIN BOUNDARY

SPACE LATTICE SYMMETRY

(1) MIRROR PLANE

(2) ROTATIONAL SYMMETRY (n-FOLD)

n = NUMBER OF EQUAL ANGLES OF ROTATION TO GET BACK TO ORIGINAL CONFIGURATION (EACH ROTATION MUST YIELD ORIGINAL CONFIGURATION)

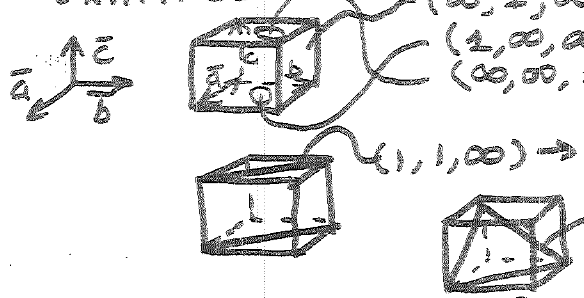
EXAMPLE: CUBIC CRYSTALS: FOUR 3 FOLD ROTA. AXES

B) MILLER INDICES (CRSTAL CONFIGURATION)

(1) FIND THE PLANE INTERCEPTS WITH $\bar{a}$, $\bar{b}$, AND $\bar{c}$ AS INTEGRAL MULTIPLES AND RECIPROCATE

(2) CLEAR FRACTIONS, RESULT: (h, k, ℓ)

EXAMPLE



$(\infty, 1, \infty) \rightarrow (0,1,0)$

$(1, \infty, \infty) \rightarrow (1,0,0)$

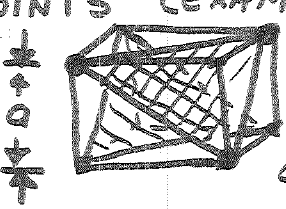
$(\infty, \infty, 1) \rightarrow (0,0,1)$

$(1, 1, \infty) \rightarrow (1,1,0)$

$(1,1,1) \rightarrow (1,1,1)$

THE PLANE WILL INTERSECT THE ~~PLANE~~ CELL @ $\bar{a}/h$, $\bar{b}/k$, AND $\bar{c}/\ell$

SPACING BETWEEN PLAINS CONTAINING LATTICE POINTS (EXAMPLES)



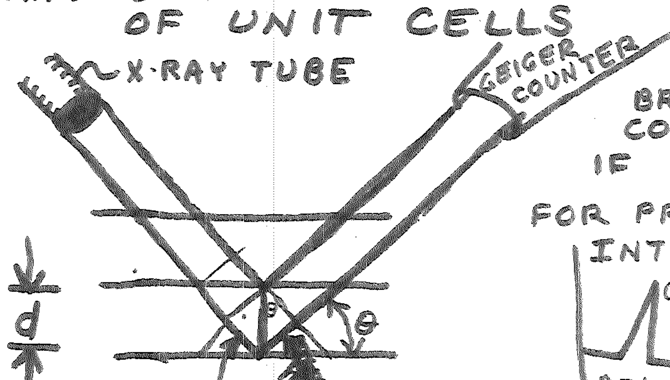
$(1,0,0)$; $d = a$

$(1,1,0)$; $d = a/\sqrt{2}$

$(1,1,1)$; $d = a/\sqrt{3}$

GENERALLY; $d = a\,(h^2 + k^2 + \ell^2)^{-1/2}$

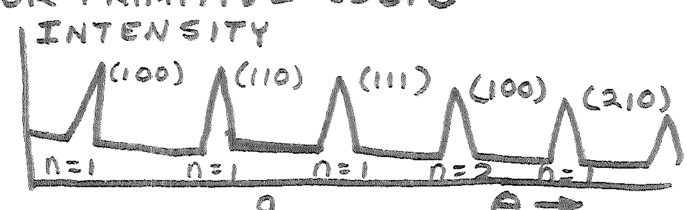
C) X-RAY DETERMINATION (BY DIFFRACTION) OF UNIT CELLS



BRAGG'S LAW FOR CONSTRUCTIVE INTERFERENCE:

IF $2d \sin\theta = n\lambda$: CONSTR. INTER.

FOR PRIMITIVE CUBIC

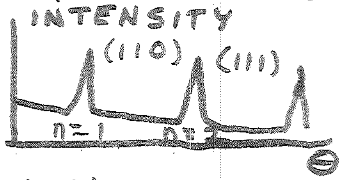


$$d = \frac{a}{\sqrt{h^2+k^2+\ell^2}}$$

$$\Rightarrow \sin\theta = \frac{n\lambda\sqrt{h^2+k^2+\ell^2}}{2a}$$

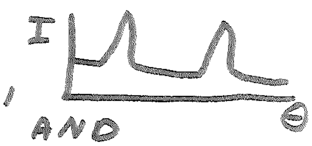
$$\Rightarrow \text{LATTICE CONSTANT: } a = \frac{n\lambda\sqrt{h^2+k^2+\ell^2}}{2\sin\theta}$$

FOR BODY CENTERED CUBICS:



(KNOCKS OUT EVERY OTHER PEAK)

$n\cdot(hkl)$	CUBIC PRIMITIVE	CUBIC BODY CENTER	CUBIC FACE CENTER
100	✓	—	✓
110	✓	✓	—
111	✓	—	—
200	✓	✓	✓
210	✓	—	✓
211	✓	✓	—
220	✓	✓	—
221	✓	—	✓



DETERMINATION OF CRYSTAL GIVEN λ AND 2θ,

1) ASSUME FIRST PEAK IS (100)... COMPUTE a AND SEE IF THE OTHER PEAKS FIT WITH a AND SOME hkl
2) ASSUME BCC $\Rightarrow$ FIRST PEAK @ (110) $\Rightarrow$ . . .
3) ASSUME FCC $\Rightarrow$ FIRST PEAK @ (111) $\Rightarrow$ . . .

⋮

IV) IONIC CRYSTALS

$Na^+Cl^- \Rightarrow$ CUBE OF VOLUME R^3 CONTAINS $\frac{1}{2}Na$ AND $\frac{1}{2}Cl$

FOR N ION PAIRS: $V = 2NR^3$

FOR OTHER CRYSTALS:

$$V = CNR^3$$

FOR 2 IONS: $E = E_a$ (ATTRACTION OR COULOMB) $+ E_r$ (REPULSION OR EXCLUSION)

$$E_a = \frac{q_1 q_2}{4\pi\epsilon_0 r_{12}}$$

ION # 1 (SODIUM IN CENTER)

$$E_{a_1} = \frac{1}{4\pi\epsilon_0}\left(\cancel{\frac{q_1 q_2}{4\pi\epsilon}}\ \frac{q_1 q_2}{r_{12}} + \frac{q_1 q_3}{r_{13}} + \frac{q_1 q_4}{r_{14}} + \dots\right)$$

$$E_{c_1} = -\frac{e^2}{4\pi\epsilon_0 R}\left(\frac{6}{1} - \frac{12}{\sqrt{2}} + \frac{8}{\sqrt{3}} - \dots\right)$$

INCLUDING ONLY THE PART OF THE ATOM INSIDE THE CUBE (EVJEN METHOD OF CUTTING OFF THE SERIES):

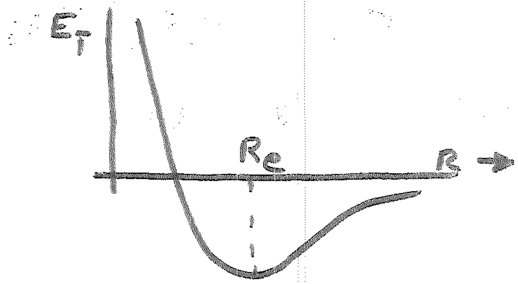
$$E_{c_1} = \frac{-e^2}{4\pi\epsilon_0}\left(\frac{3}{1} - \frac{3}{\sqrt{2}} + \frac{1}{\sqrt{3}} - \dots\right)$$

$$= -\alpha e^2 / 4\pi\epsilon_0 R$$

α = MODELING CONSTANT ($= 1.747$ FOR NaCl)

TOTAL P.E:

$$E_T = N\left[\frac{-\alpha e^2}{4\pi\epsilon_0 R} + \frac{A}{R^n}\right]$$



$$\left.\frac{\delta E_T}{\delta R}\right|_{R=R_e} = 0 \quad \Rightarrow T = 0^\circ K$$

$$\Rightarrow E_{T_0} = \frac{-N\alpha e^2}{4\pi\epsilon_0 R_e}\left[1 - \frac{1}{n}\right]$$

$\ni n$ IS RELATED TO COMPRESSIBILITY (K)

$$\frac{dW}{dt} = -p\,dV = dE \Rightarrow \frac{dp}{dV} = \frac{-dE^2}{dV^2}$$

$$\frac{1}{K} = \frac{-1}{V}\frac{dV}{dP} \Rightarrow \frac{1}{K} = -V\frac{dp}{dV} = V\frac{d^2E}{dV^2}$$

$$\frac{d^2E}{dt^2} = \frac{dE}{dR}\frac{\delta}{\delta V}\left(\frac{\delta R}{\delta V}\right) + \frac{dR}{dV}\frac{\delta}{\delta V}\left(\frac{\delta E}{\delta R}\right) = \frac{dE}{dR}\frac{d^2R}{dV^2} + \frac{d^2E}{dR^2}\left(\frac{dR}{dV}\right)^2$$

$$\Rightarrow \frac{1}{K_0} = V\frac{d^2E}{dR^2}\left[\frac{dR}{dV}\right]^2$$

VOLUME OF CRYSTAL: $V = CNR^3$

$$\Rightarrow \frac{dV}{dR} = 3CNR^2$$

$$\Rightarrow \frac{1}{K_0} = CNR_e^3\,\frac{d^2E}{dR^2}\left[\frac{1}{9C^2N^2R_e^4}\right]$$

$$= \frac{1}{9CNR_e}\left.\left(\frac{d^2E}{dR^2}\right)\right|_{R=R_e}$$

NOW $\Rightarrow \left.\frac{d^2E}{dR^2}\right|_{R=R_e} = \frac{N\alpha e^2}{4\pi\epsilon_0}\left[\frac{n-1}{R_e^3}\right]$

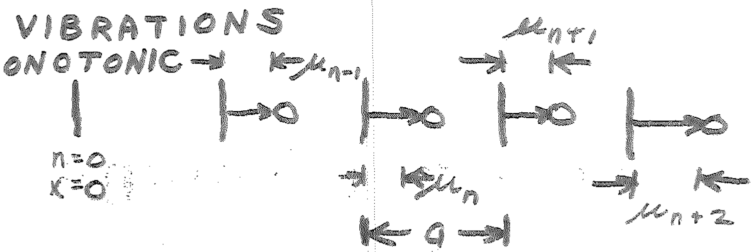
$$\Rightarrow \frac{1}{K_0} = \frac{1}{9CNR_e}\left[\frac{N\alpha e^2}{4\pi\epsilon_0}\left(\frac{n-1}{R_e^3}\right)\right]$$

$$= \alpha e^2(n-1)/36\pi C\epsilon_0 R_e^4$$

SOLVE FOR n.

VIBRATIONS

① MONOTONIC



CONSIDER FORCES BETWEEN ATOMS:

$$F_n = \beta(\mu_{n+1} - \mu_n) - \beta(\mu_n - \mu_{n-1})$$

$$M\ddot{\mu}_n = \beta(\mu_{n+1} + \mu_{n-1} - 2\mu_n) \rightarrow \text{WAVE EQUATION}$$

$$\therefore \mu = \mu_0 e^{i(\omega t - kx)} \ni \omega = 2\pi f,\ k = 2\pi/\lambda$$

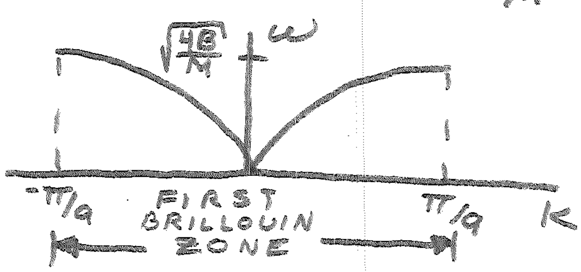
$$\text{or } \mu_n = \mu_0 e^{i(\omega t - kna)} \ni x = na$$

$$\Rightarrow -\omega^2 M \mu_0 e^{i(\omega t - kna)} = \beta \mu_0 e^{i(\omega t - kna)}\left[e^{ika} + e^{-ika} - 2\right]$$

$$\text{ALSO } e^{ika} + e^{-ika} + 2 = \left(e^{ika/2} - e^{-ika/2}\right)^2 = -4\sin^2 ka/2$$

$$\Rightarrow \omega^2 M = -4\beta \sin^2 \frac{ka}{2}$$

$$\therefore \omega = \sqrt{\frac{4\beta}{M}} \sin \frac{ka}{2}$$



V_p = PHASE SPEED = $f/\lambda = \omega/k$

V_g = GROUP VELOCITY = $\delta\omega/\delta k$

② DIATONIC

TWO D.E.'S

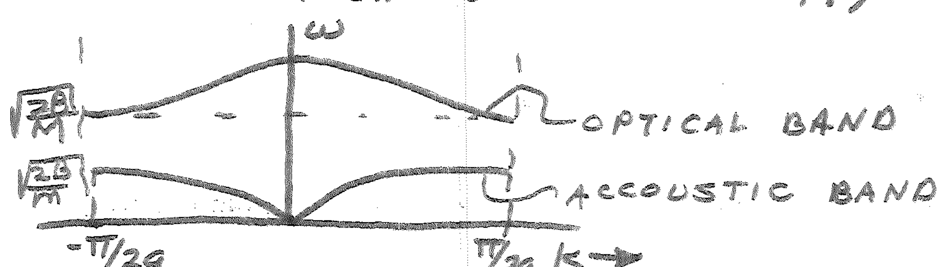
$$M\ddot{\mu}_{2n} = \beta(\mu_{2n} + \mu_{2n+2} - 2\mu_{2n})$$

$$m\ddot{\mu}_{2n+1} = \beta(\mu_{2n} + \mu_{2n+2} - 2\mu_{2n+1})$$

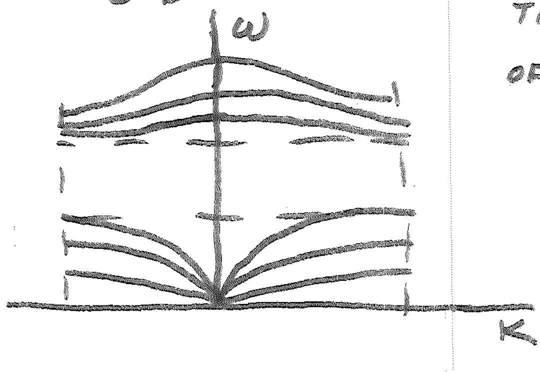
$$\Rightarrow \mu_{2n} = \xi e^{i(\omega t + 2nka)}$$

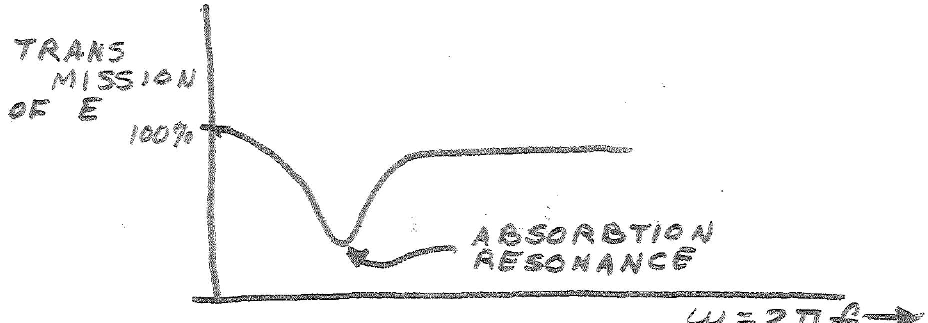
$$\mu_{2n+1} = \eta e^{i(\omega t + (2n+1)ka)}$$

$$\text{THEN } \omega^2 = \beta\left(\frac{1}{m} + \frac{1}{M}\right) \pm \beta\left[\left(\frac{1}{M} + \frac{1}{m}\right)^2 - \frac{4\sin^2 ka}{Mm}\right]^{\frac{1}{2}}$$

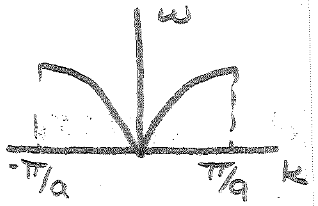


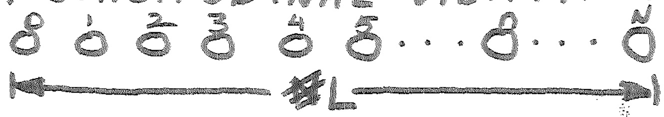
IN 3-D





MONATONIC LATTICE: LONGITUDINAL VIBRATIONS





0 AND N ARE FIXED

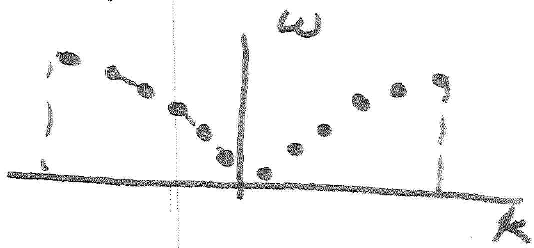
$\Rightarrow \sin kL = \sin kNa = 0 \Rightarrow kL = kNa = 2m\pi$

STANDING WAVE EQUATION:

$u = Re[u_0 e^{i\omega t} \sin kx]$

$\therefore k = \frac{\pi}{L}, \frac{2\pi}{L}, \frac{3\pi}{L}, \ldots, \frac{(n-1)\pi}{L}$

@ $k = \frac{n\pi}{L}$, $u = 0$



$\therefore$ DISCRETE k & ω

V) SPECIFIC HT. ON INSULATORS

A) CLASSICAL STATISTICAL MECHANICS

1) PHASE SPACE; $d\Omega = dx\,dy\,dz\,dp_x\,dp_y\,dp_z$

2) EQUALIBRIUM DISTRIBUTION = MOST PROBABLE DISTRIBUTION OF POINTS AMONG CELLS

EXAMPLE: 2 BOXES; 4 PARTICLES

a) ALL IN CELL A $\longrightarrow$ 1 WAY

b) 3 IN A, 1 IN B $\longrightarrow$ 4 WAYS

c) 2 IN A, 2 IN B $\longrightarrow$ 6 WAYS

$\Rightarrow P = N! / \prod_{i=1} N_i! \ni \sum_{i=1} N_i = N$ AND $N_i \in P.I.$

3) MAXWELL BOLTZMAN DISTRIBUTION:

$dN \propto e^{-E_i/kT} d\Omega$

FRACTION OF PARTICLES @ $P(P_x, P_y, P_z)$ AND POSITION X, Y, Z IN PHASE SPACE $d\Omega$

$$= \frac{dN}{N} = e^{-E/kT} d\Omega \int_{-\infty}^{\infty}\!\!\int e^{-E/kT} d\Omega$$

$$= \frac{P_x^2 + P_y^2 + P_z^2}{2m} + \tfrac{1}{2}B(X^2+Y^2+Z^2)$$

$$\bar{E} = \frac{\int E\,dN}{N} = \frac{\int E\,e^{-E/kT} d\Omega}{\int e^{-E/kT} d\Omega} = 3kT$$

TOTAL E ON N VIBRATING ATOMS: $U = 3NkT$

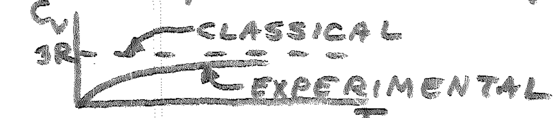
FOR 3 GRAM MOLES:

$U = 3N_0 kT = 3RT$

N_0 = AVAGADRO'S NUMBER

R = IDEAL GAS CONSTANT

4) SPECIFIC HT/PER MOLE $= C_v = \left.\frac{\delta Q}{\delta T}\right|_v = \left.\frac{\delta U}{\delta T}\right|_v = 3R = 5.96 \frac{\text{CALORIES}}{\text{MOLE}\,°K}$



FROM QUANTUM MECHANIC OSCILLATORS

$E = (n + \tfrac{1}{2})hf$; $n = 0, 1, 2, \ldots$

B) EINSTEIN MODEL OF THE ATOM

1) ASSUMPTIONS

a) ALL ATOMS VIBRATE WITH SINGLE FREQUENCY f

b) EACH OSCILLATOR IS 3 LINEAR HARMONIC OSCILLATORS (MUTUALLY $\perp$ VIBRATIONS

c) N ATOMS $\longrightarrow$ 3N LINEAR OSCILLATORS

d) BOLTZMAN DISTRIBUTION: $N_i \propto e^{E_i/kT}$

WITH $U = 3N\bar{E} \ni \bar{E}$ = AVERAGE ENERGY

2) DERIVATION

$$N_i \propto e^{-E_i/kT}$$

$$\bar{E} = \sum_i E_i e^{-E_i/kT} \Big/ \sum_i e^{-E_i/kT}$$

$$= \sum_{n=0}^{\infty} (n+\tfrac{1}{2}) hf \exp\left[-(n+\tfrac{1}{2}) hf/kT\right] \Big/ \sum_{n=0}^{\infty} e^{-(n+\frac{1}{2})hf/kT}$$

$$= \frac{e^{-\frac{1}{2}hf/kT}}{e^{-\frac{1}{2}hf/kT}} \sum_{n=0}^{\infty} (n+\tfrac{1}{2}) hf\, e^{-nhf/kT} \Big/ \sum_{n=0}^{\infty} e^{-nhf/kT}$$

$$= \frac{\frac{hf}{2}\sum_{n=0}^{\infty} e^{-nhf/kT}}{\sum_{n=0} e^{-nhf/kT}} + \frac{\sum_{n=0}^{\infty} nfh \exp\left(\frac{-nhf}{kT}\right)}{\sum_{n=0}^{\infty} e^{-nhf/kT}}$$

$$= \tfrac{1}{2}hf + \frac{hf\, e^{-\frac{hf}{kT}} + 2hf\, e^{-\frac{2hf}{kT}} + 3hf\, e^{-3hf/kT} + \dots}{1 + e^{-hf/kT} + e^{-2hf/kT} + \dots}$$

LET $x = -hf/kT$

$$\Rightarrow \bar{E} = \tfrac{1}{2}hf + hf\left[\frac{e^{x} + 2e^{2x} + 3e^{3x} + \dots}{1 + e^{x} + e^{2x} + \dots}\right]$$

LET $U = 1 + e^{x} + e^{2x} + \dots = 1/1-e^{x}$ (DENOMINATOR)

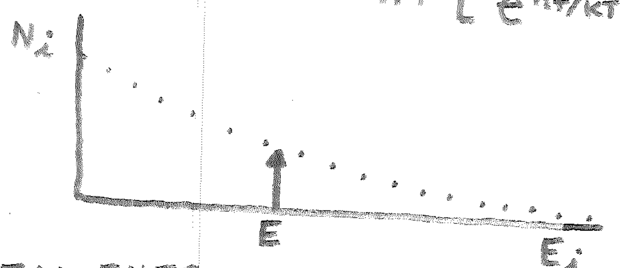
$\Rightarrow dU = e^{x} + 2e^{2x} + 3e^{3x} + \dots$ = NUMERATOR

NOW $\frac{d}{dx}\left[\frac{1}{1-e^{x}}\right] = \frac{e^{x}}{(1-e^{x})^2}$

THUS: $\bar{E} = \tfrac{1}{2}hf + hf\,\frac{(1-e^{x})^{-2}e^{x}}{(1-e^{x})^{-1}}$

$$= \tfrac{1}{2}hf + hf\left[\frac{e^{x}}{1-e^{x}}\right] = \tfrac{1}{2}hf + hf\left[\frac{1}{e^{-x}-1}\right]$$

$$= \tfrac{1}{2}hf + hf\left[\frac{1}{e^{hf/kT}-1}\right]$$



TOTAL ENERGY

$$U = 3N\bar{E} = \tfrac{3}{2}Nhf + 3Nhf\left[\frac{1}{e^{hf/kT}-1}\right]$$

$$C_v = \frac{\delta U}{\delta T}\Big]_v = 3Nhf\,\frac{\delta}{\delta T}(e^{hf/kT}-1)^{-1}$$

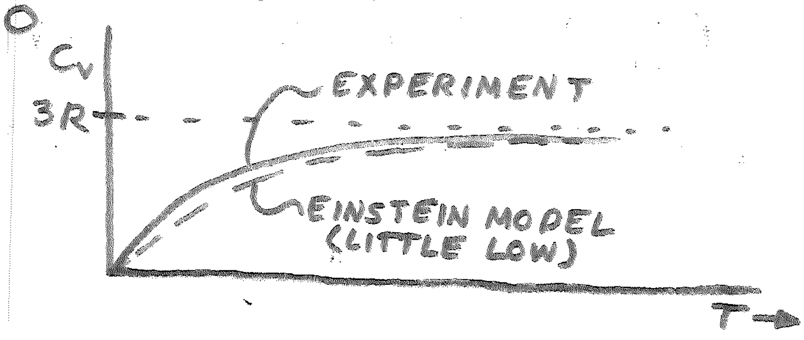
$$= \frac{3N}{k}\left[\left(\frac{hf}{T}\right)^2 \frac{e^{hf/kT}}{(e^{hf/kT}-1)^2}\right]$$

FOR 1 MOLE ($N = N_0$)

$$C_v = 3R\left[\left(\frac{hf}{kT}\right)^2 e^{hf/kT} \Big/ (e^{hf/kT}-1)^2\right]$$

@ $T = \infty$, $e^{hf/kT} = 1$; $\Rightarrow C_v = 3R$

@ $T = 0$, $C_v = 0$



C) DEBYE MODEL

1) ASSUMPTIONS

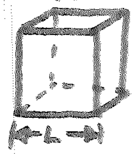
(a) 3N LINEAR HARMONIC OSCILLATORS

(b) MAXWELL DISTRIBUTION

(c) FREQUENCY ASSUMPTIONS

(1) STANDING WAVES OF CONTINUOUS MEDIUM

(2) ALL WAVES TRAVEL @ THE SAME SPEED (NON-DISPERSIVE MEDIA)



$L = n\lambda/2 \ni n = 1, 2, 3, \ldots$

$f = V/\lambda$

2) DERIVATION

WAVE EQUATION: $\nabla^2 U = \frac{1}{V^2}\frac{\delta^2 U}{\delta t^2} = \frac{\delta^2 U}{\delta x^2} + \frac{\delta^2 U}{\delta y^2} + \frac{\delta^2 U}{\delta z^2}$

$\Rightarrow \mu = \mu_0 \sin\left(\frac{n_x \pi x}{\ell}\right)\sin\left(\frac{n_y \pi y}{\ell}\right)\sin\left(\frac{n_z \pi z}{\ell}\right)\cos(2\pi f t)$

$\ni n_x, n_y, n_z = 1, 2, 3, 4, \ldots$

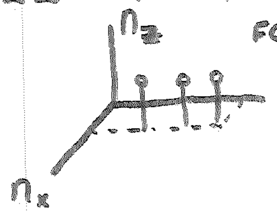
PLUGGING BACK INTO THE WAVE EQUATION:

$-\left(\frac{n_x \pi}{\ell}\right)^2 \mu - \left(\frac{n_y \pi}{\ell}\right)^2 \mu - \left(\frac{n_z \pi}{\ell}\right)\mu = \frac{1}{V^2}(2\pi f)^2 \mu$

$-\left(\frac{\pi}{\ell}\right)^2 (n_x^2 + n_y^2 + n_z^2) = 4\pi^2 f^2/V^2$

$\Rightarrow f =$ STANDING WAVE FREQUENCIES

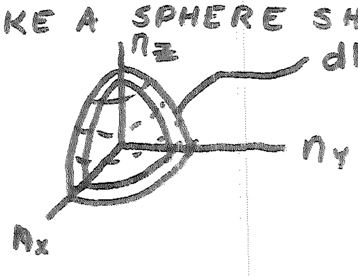
$= \frac{V}{2\ell}\sqrt{n_x^2 + n_y^2 + n_z^2} = \frac{V}{2\ell} R$



FORMS CUBIC "LATTICE" EACH POINT REPRESENTING A STANDING WAVE NODE

$\therefore R = 2\ell f / V$ AND $dR = \frac{2\ell}{V} df$

TAKE A SPHERE SHELL



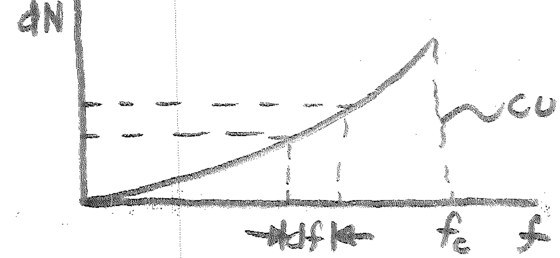
$dN = \frac{1}{8}(4\pi R^2) dR$

$= \frac{\pi}{2} R^2 dR$

$= \frac{\pi}{2}\left(\frac{4\ell^2 f^2}{V^2}\right)\left(\frac{2\ell}{V} df\right)$

$= \frac{4\pi \ell^3}{V^3} f^2 df$

$= \frac{4\pi \mathbb{V}}{V^3} f^2 df \ni \mathbb{V} = \ell^3 =$ CUBE'S VOLUME



3 VIBRATIONS
TWO TRANSVERSE, WITH VELOCITY V_T
ONE LONGITUDINAL, WITH VELOCITY V_ℓ

$$\Rightarrow dN = 4\pi V\left(\frac{2}{V_t^3}+\frac{1}{V_\ell^3}\right)f^2 df$$

NOW $3N = \int_0^{f_d} dN \ni f_d =$ CUT OFF FREQUENCY

$$= 4\pi V\left(\frac{2}{V_t^3}+\frac{1}{V_\ell^3}\right)\int_0^{f_d} f^2 df$$

$$\Rightarrow f_0 = \left[\frac{9N}{4\pi V}\left(\frac{2}{V_t^3}+\frac{1}{V_\ell^3}\right)^{-1}\right]^{\frac{1}{3}}$$

IF EACH OSCILLATOR HAS THE AVERAGE ENERGY OF EINSTEIN'S OSCILLATORS:

$$\overline{E} = hf/(e^{hf/KT}-1)$$

THEN TOTAL ENERGY

$$U = \int_0^{f_0} E\, dN$$

$$= \int_0^{f_0}\left(\frac{hf}{e^{hf/KT}-1}\right)dN$$

$$= 4\pi V\left(\frac{2}{V_t^3}+\frac{1}{V_\ell^3}\right)\int_0^{f_0}\frac{hf^3}{e^{hf/KT}-1}df$$

SUBSTITUTING $\left(\frac{2}{V_t^3}+\frac{1}{V_\ell^3}\right)$ FROM EXPRESSION FOR f_0, LETTING $X = hf/KT$ AND $X_0 = hf_0/KT$

$$\Rightarrow 9N\left(\frac{KT}{hf_0}\right)^3 KT\int_0^{X_0}\frac{x^3dx}{e^x-1} = U$$

① FOR HI T

$$U \simeq 9N\left(\frac{KT}{hf_0}\right)^3\int_0^{X_0}\frac{x^3dx}{(x+1)-x} \simeq e^x \cong 1+X \simeq 3NKT = 3RT \ \frac{\text{JOULS}}{\text{MOLE}}$$

$$\Rightarrow C_V = \left.\frac{\delta U}{\delta T}\right|_V = 3R$$

② FOR LOW T ($\Rightarrow$ HI $X_0 \cong \infty$)

$$U \cong 9T\left(\frac{KT}{hf_0}\right)^3 KT\int_0^{\infty}\frac{x^3dx}{e^x-1};\ \text{BUT}\int_0^{\infty}\frac{x^3dx}{e^x-1} = \pi^4/15$$

$$\Rightarrow U \cong \frac{3}{5}\pi^4 NKT\left(\frac{T}{\Theta_D}\right)^3 \ni \Theta_D = hf_0/_K = \text{DEBYE TEMP}$$

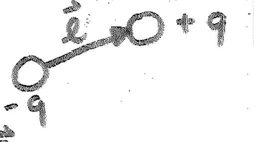
$$\Rightarrow C_V = \left.\frac{\delta U}{\delta T}\right|_V = \frac{R}{5}\pi^4 R\left(\frac{T}{\Theta_0}\right)^3$$

A GOOD FIT OF EXPERIMENTAL RESULTS. Θ_D CHOSEN TO FIT CURVE, AND DEPENDS ON THE SUBSTANCE

VI) DIELECTRICS

A) DEFINITIONS OF $\vec{p}, \vec{P}, \vec{D}, K, \alpha$

1) $\vec{p}$ = DIPOLE MOMENT



$\vec{p} = q\vec{\ell}$

2) $\vec{P}$ = POLARIZATION: $\vec{P} = \frac{\sum p_i}{V} = \frac{\text{DIPOLE MOMENT}}{\text{UNIT VOLUME}}$

3) $\vec{D}$ = DISPLACEMENT: $\vec{D} = \epsilon_0 \vec{E} + \vec{P}$

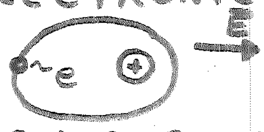
⇒ DIELECTRIC DECREASES $\vec{E}$ IF CHARGE ON THE PLATES IS THE SAME

4) K = DIELECTRIC CONSTANT

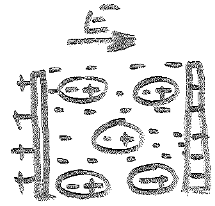
$$\vec{D} = K\epsilon_0\vec{E} = \epsilon_0\vec{E} + \vec{P} \Rightarrow K = 1 + \frac{P}{\epsilon_0 E}$$

B) TYPES OF POLARIZATION

1) ELECTRONIC POLARIZATION



SHIFT e^- ORBITS RELATIVE TO NUCLEUS

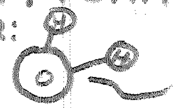


POLARAZATION IN DIELECTAIC

2) IONIC POLARIZATION

3) ORIENTATIONAL POLARIZATION

WATER:



DIPOLE

REORIENTATION OF PERMANENT DIPOLE ON $\vec{E}$

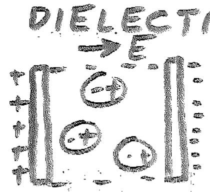
C) LOCAL FIELDS DUE TO DIPOLES AND OTHER CHARGES AT THE ATOMIC POSITION

1) IN INSULATORS: $C_V = \left[\left(\frac{\delta U}{\delta T}\right)^{VIB}\right]_V$

IN METALS $C_V = \left[\left(\frac{\delta U_{VIB}}{\delta T}\right) + \left(\frac{\delta U_{ELEC}}{\delta T}\right)\right]_V = (C_V)_{VIB} + (C_V)_{ELEC}$

$P = \hbar k \ni k = 2\pi/\lambda$; P = PHONON VIBRATION

IN DIELECTRIC

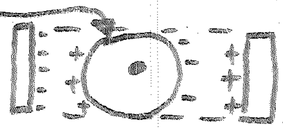


E_{loc} = LOCAL FIELD @ POSITION OF ATOM DUE TO OTHER CHARGES

E_1 = E FIELD @ PT. DUE TO PLATES

E_2 = E FIELD @ PT. DUE TO OUTSIDE PLATE POLARIZATION CHARGE ⇒ $\bar{E} = E_1 + E_2$

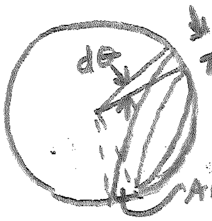
$\bar{E}_3$ = E FIELD DUE TO CHARGE ON CAVITY SURFACE



E_4 = E FIELD INSIDE THE CAVITIES DUE TO INDIVIDUAL DIPOLES

$$\Rightarrow \bar{E}_{loc} = \bar{E}_1 + \bar{E}_2 + \bar{E}_3 + \bar{E}_4$$
$$= \bar{E} + \bar{E}_3 + \bar{E}_4$$

2) E_3: DUE TO CAVITY SURFACE



$-\oint \vec{P}\cdot d\vec{S} = q_{POL}$ (ENCLOSED)

$= \sigma_p\, dS = -P\cos\theta\, dS$

$\Rightarrow \sigma_p$ = SURFACE DENSITY $= -P\cos\theta$

AREA $= R\,d\theta\; 2\pi R\, \cancel{\cos}\,\sin\theta$

$\Rightarrow dq = -\sigma(2\pi R^2 \sin\theta)\,d\theta$

$dE_3 = \frac{-1}{4\pi\epsilon_0}\frac{dq}{r^2}\cos\theta$

$E_3 = \frac{-P}{2\epsilon_0}\int_0^{\pi} \cos^2\theta \sin\theta\, d\theta$

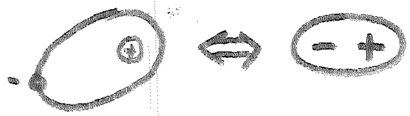
$= \frac{-P}{2\epsilon_0}\,\frac{\cos^3\theta}{3}\Big|_0^{\pi} = \frac{P}{3\epsilon_0}$

$\therefore E_{loc} = E + \frac{P}{3\epsilon_0} + E_4$

FOR A CUBIC LATTICE; $E_4 = 0$

FOR OTHER LATTICE; $E_4 = \gamma_j P$

D) ATOM IN $\vec{E}$ FIELD (CLAUSUIS-MOSSATI)



ATOMIC POLARIZABILITY; $\alpha_i = \frac{p}{E_{loc}} \ni p$ = DIPOLE MOMENT

FOR CUBIC LATTICE OF IDENTICAL ATOMS

$E_{loc} = E + P/3\epsilon_0$; $\left.\begin{array}{l}\vec{D} = K\epsilon_0\vec{E}\\ \vec{D} = \epsilon_0\vec{E} + P\end{array}\right\} K = 1 + \frac{P}{\epsilon_0 E}$

$K = 1 + \frac{P}{\epsilon_0 E} \Rightarrow P = (K+1)\epsilon_0 E$

$E_{loc} = E + (K-1)\frac{E}{3}$

$= \left(\frac{K+2}{3}\right)E$

AND $K-1 = \frac{P}{\epsilon_0 E_{loc}\left(\frac{3}{K+2}\right)} \Rightarrow \frac{K-1}{K+2} = \frac{P}{3\epsilon_0 E_{loc}}$ $\Big\{$ CLAUSUIS MOSSATI EQUATION

E) IONIC POLARIZABILITY

APPLY AN E FIELD; ~~SHM~~

SHIFT OF X IONS RELATIVE TO NEGATIVE IONS

DIPOLE MOMENT: $eE_{loc} = \beta x \Rightarrow x = eE_{loc}/\beta$

$P_{IONIC} = N x e$

$= (Ne^2/\beta)E_{loc}$

$\frac{K-1}{K+2} = \frac{P}{3\epsilon_0 E_{loc}} = \frac{N\alpha_{loc} + NE_{loc} + Ne^2E_{loc}/\beta}{3\epsilon_0 E_{loc}}$

$= \frac{N}{3\epsilon_0}\left[x_i + \frac{e}{\beta} + \quad\right]$

$\omega = \sqrt{\beta/m}$

F) ORIENTATIONAL POLARIZATION

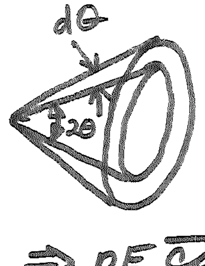
ALIGNMENT OF PERMANENT DIPOLES WITH E FIED PRESENT TENDS TO LINE UP DIPOLES, WHILE INTERACTIONS 'TWIXT THE DIPOLES THEMSELVES TEND TO RANDOMIZE DIRECTION

$$U = -p \cdot \bar{E} = -pE\cos\theta$$

$$\bar{U} = \frac{1}{N}\int U\,dN$$

$$= \frac{-\int pE\cos\theta\, e^{pE\cos\theta/kT}\,d\Omega}{\int e^{pE\cos\theta/kT}}$$

$$\ni e^{-U/kT} = e^{pE\cos\theta/kT}$$



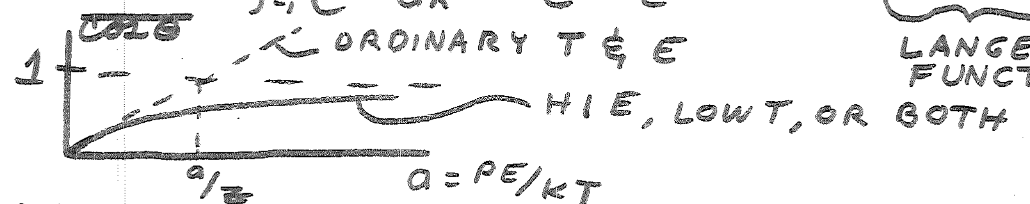
$d\Omega$ IS THE SOLID ANGLE 'TWIXT θ AND $d\theta$

$$d\Omega = \frac{\text{AREA SUBT. ON SPHERE}}{R^2}$$

$$\Rightarrow pE\overline{\cos\theta} = \frac{\int_0^\pi pE\cos\theta\, e^{pE\cos\theta/kT}\, 2\pi\sin\theta\, d\theta}{\int_0^\pi e^{pE\cos\theta/kT}\, 2\pi\sin\theta\, d\theta}$$

NOW $dx = -\sin\theta\, d\theta \Rightarrow x = \cos\theta$; LET $a = pE/kT$

$$\Rightarrow \overline{\cos\theta} = \frac{\int_{-1}^{1} x\, e^{ax}dx}{\int_{-1}^{1} e^{ax}dx} = \frac{e^a + e^{-a}}{e^a - e^{-a}} - \frac{1}{a} = \underbrace{\coth a - \frac{1}{a}}_{\text{LANGEVIN FUNCTION}}$$



FOR NORMAL T & E, $a \ll 1$, AND $\overline{\cos\theta} \cong a/3$

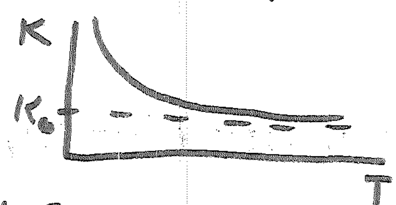
THEN $P = Np\overline{\cos\theta} \ni N =$ DIPOLES/VOLUME

$$= Np\frac{pE}{3kT} = Np^2E/3kT$$

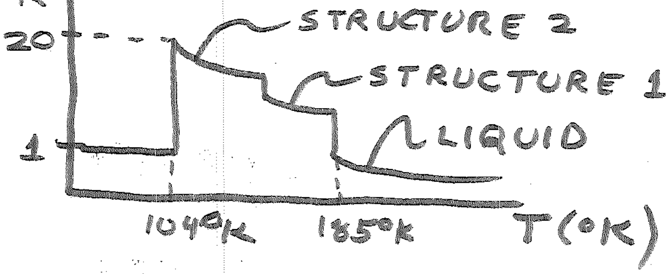
NOW $K_0 = 1 + P/\epsilon_0 E = 1 + Np^2/3\epsilon_0 kT$

IF OTHER POLARIZATION IS THERE

$K = K_0 + C/T$ (CURIE LAW)



FOR H_2S



G) A-C $\vec{E}$ FIELDS IN A DIELECTRIC

$$E = E_0 e^{i\omega t}$$

$$\Sigma F = m\frac{d^2x}{dt^2} = qE_0 e^{i\omega t} - \beta x - m\gamma\frac{dx}{dt}$$

β = RESTORING COEFFICIENT

γ = FUDGE FACTOR

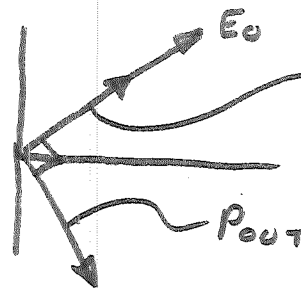
$m\gamma\frac{dx}{dt}$ = RADIATION LOSS

BY MAGIC:

$$x = \frac{q}{m}\left[\frac{E_0 e^{i\omega t}}{\omega_0^2 - \omega^2 + i\gamma\omega}\right] = \frac{qE_0}{m}e^{i\omega t}\left[\frac{\omega_0^2 - \omega^2 - i\gamma\omega}{(\omega_0^2 - \omega^2) + \gamma^2\omega^2}\right]$$

$$= \frac{qE_0}{m}e^{i\omega t}\left\{\left[\frac{\omega_0^2 - \omega^2}{(\omega_0^2 - \omega^2) + \gamma^2\omega^2}\right] - i\left[\frac{\gamma\,\omega}{(\omega_0^2 - \omega^2) + \gamma^2\omega^2}\right]\right\}$$

NOW $p = qx \Rightarrow P = Nqx = \frac{Nq^2E_0}{m}e^{i\omega t}$



1) FOR A SLOW FIELD ($\omega << \omega_0$)

$P_{IN} = \frac{Nq^2E_0}{m}e^{i\omega t}\left(\frac{1}{\omega^2}\right)$ ∴ ($\gamma^2\omega^2$ IS NEGLIGIBLE)

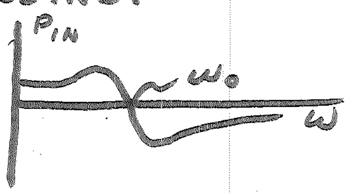
$P_{OUT} = 0$

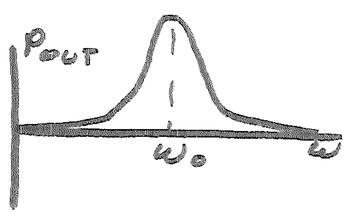
2) NEAR $\omega = \omega_0$

$P_{IN} = 0$

$P_{OUT} = \frac{Nq^2E_0}{m\gamma\omega}e^{i\omega t}$

YIELDING:





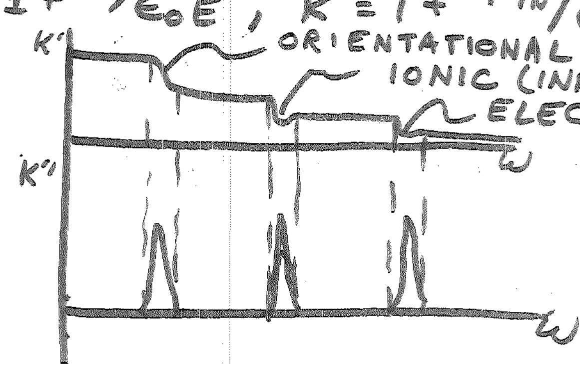
3) FOR $\omega >> \omega_0$, $P_{IN} = \frac{Nq^2E_0 e^{i\omega t}}{\omega}\left[\frac{-\omega^2}{\omega^4 + \gamma^2\omega^2}\right] \Rightarrow 0$

SIMILARLY $P_{OUT} \rightarrow 0$

$PWR = \frac{dw}{dt} = FV$;

POWER INPUT MAXIMUM @ $\omega = \omega_0$

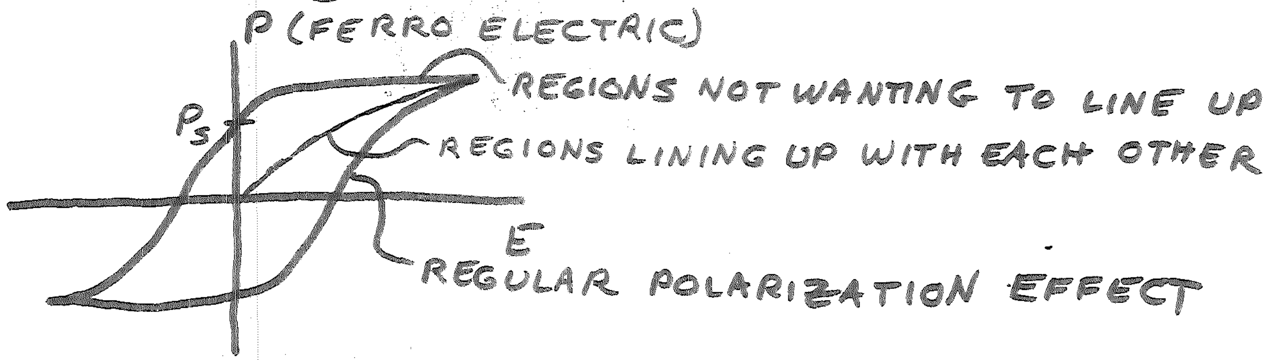
$K = 1 + P/\epsilon_0 E$; $K' = 1 + P_{IN}/\epsilon_0 E$; $K'' = 1 + P_{OUT}/\epsilon_0 E$

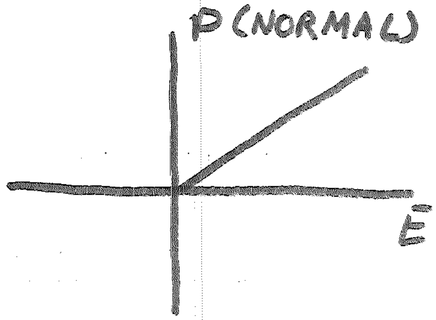


H) FERRO-ELECTRICITY

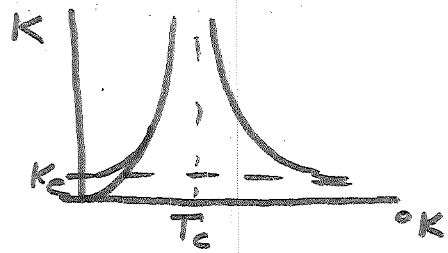
a) UNIT CELLS HAVE NO INVERSION CENTER OF SYMMETRY
b) ALTERNATING POSITIONS FOR SOME ATOMS IN UNIT CELL
c) DIPOLE IN ONE CELL IS STRONG ENOUGH TO PRODUCE DIPOLE IN NEXT, ETC. (CO-OPERATIVE PHENOMENON)
d) ⇒ POLARIZATION WITH ALL DIPOLE MOMENTS IN A GIVEN REGION OF CRYSTAL (DOMAIN) ARE IN THE SAME DIRECTION

APPLYING $\bar{E}$ FIELD





$$K = 1 + \frac{P}{\epsilon_0 E} = 1 + \frac{1}{\epsilon_0} \left.\frac{dP}{dE}\right|_{E=0}$$



$$K = K_e + \frac{C}{T - T_c}$$

T_c = CURIE TEMPERATURE

III) ATOMIC DIAMAGNETISM AND ATOMIC FERROMAGNETISM

A) MAGNETIC PROCESSES

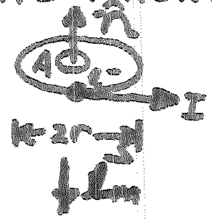
APPLICATION OF $\vec{H}$ TO A MATERIAL INDUCES A MAGNETIZATION $\vec{M}$

$$\vec{M} = \Sigma P_m/V = \mu \vec{H} = \mu_0 \vec{H} + M = (\mu_0 + \chi)\vec{M}$$

WHERE $\chi = M/H$ = MAGNETIC SUSCEPTIBILITY

B) MAGNETIC MOMENTS

1) ORBITAL MAGNETIC MOMENT (FOR A CIRCLE)



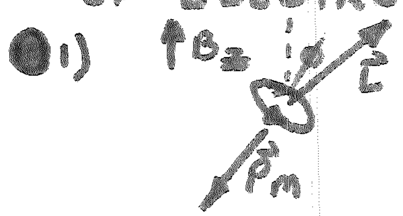
$$\vec{P}_m = IA\hat{n}$$
$$= \left(\frac{ev}{2\pi r}\right)(\pi r^2)\hat{n} = \frac{evr}{2}\hat{n}$$
$$= \frac{-e}{2m}(-mvr\hat{n})$$
$$= \frac{-e}{2m}\vec{L} \ni \vec{L} = \text{ORBITAL MAGNETIC MOMENTUM}$$

2) SPIN MAGNETIC MOMENT

$$\vec{P}_s = -g\left(\frac{e}{2m}\right)\vec{S} \ni \vec{S} = \text{SPIN ANGULAR MOMENTUM}$$
g = FUDGE FACTOR

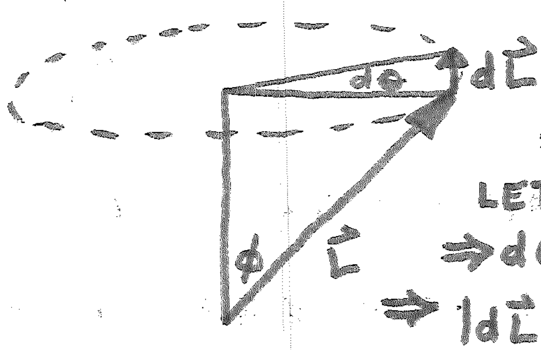
C) DIAMAGNETISM DUE TO LARMOR PRECESSION OF ELECTRON ORBIT

1)



$$\tau = \vec{P}_m \times \vec{B} = \frac{\delta \vec{L}}{\delta t}$$

ELECTRON CIRCLE WILL CHANGE ITS TILT IN TIME, MUCH AS WOULD A TOP



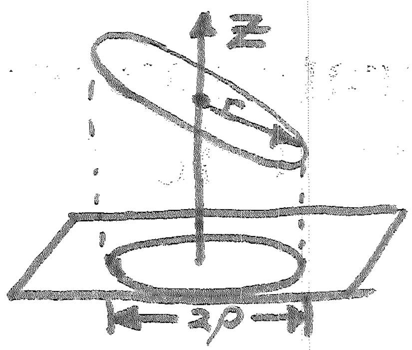
$$\tau = \vec{P}_m \times \vec{B} = \delta\vec{L}/\delta t$$
$$= -\left(\frac{e}{2m}\right)\vec{L}\times\vec{B}$$
$$\Rightarrow d\vec{L} = \left[\left(\frac{-e}{2m}\right)\vec{L}\times\vec{B}\right]dt$$

LET $\omega_L = d\theta/dt$ (LAMOR FREQ)

$$\Rightarrow d\theta = \omega_L dt = \frac{dL}{L\sin\phi}$$
$$\Rightarrow |d\vec{L}| = dL = L\sin\phi\, dt\, \omega_L$$
$$= |\vec{L}\times\vec{\omega}_L|\,dt$$

$$\Rightarrow \omega_L = \left(\frac{-e}{2m}\right)\vec{B}$$

2) INDUCED ANGULAR MOMENTUM (DIAMAGNETIC EFFECT)
-ALL IN ELECTRON'S ORBIT-



$L_{IND} = m\omega_L \rho^2$

$(\vec{P}_m)_{IND} = \frac{-e}{2m} L_{IND}$

$= \frac{-e}{2m} m\omega_L \rho^2$

SPHERE OF RADIUS r

$\left.\begin{array}{l} \overline{r^2} = \overline{x^2} + \overline{y^2} + \overline{z^2} = 3\overline{x^2} \\ \overline{\rho^2} = \overline{x^2} + \overline{y^2} \quad\quad = 2\overline{x^2} \end{array}\right\} \rightarrow \overline{\rho^2} = \frac{2}{3}\overline{r^2}$

$\Rightarrow P_{IND} = \left(\frac{-e}{2m}\right) m\omega_L \left(\frac{2}{3} r^2\right)$

ASSUME N ATOMS PER UNIT VOLUME

$M = N P_{IND}$

$\chi = M/H = N P_{IND}/H$

D) ANGULAR MOMENTUM

$|\vec{L}| = [(L+1)L]^{1/2}\hbar \ni L =$ ORBITAL ANGULAR MOMENTUM QUANTUM NUMBER $\in I$

$|\vec{S}| = [(S+1)S]^{1/2}\hbar \ni S =$ SPIN ANGULAR MOMENTUM QUANTUM NUMBER $\in I/2$

$|\vec{J}| = [(J+1)J]^{1/2}\hbar \in J =$ TOTAL ANGULAR MOMENTUM QUAUNTUM NUMBER $\in I/2$

E) ENERGY LEVELS AND THE BOHR MAGNETRON

TOTAL MAGNETIC MOMENT:

$\vec{P}_m = -g_J\left(\frac{e}{2m}\right)\vec{J} \ni g_J = 1 + \frac{J(J+1) - L(L+1) + S(S+1)}{2J(J+1)}$

APPLICATION OF $\vec{B}$ FIELD TO ATOM WITH MAGNETIC MOMENT

$J_z = Z$ COMPONENT OF J

$J_z = m_J\hbar \ni m_J = J, J-1, J-2, \ldots, -J+1, -J$

EXAMPLE: LET $J = 3/2$

$\Rightarrow m_J = 3/2, 1/2, -1/2, -3/2$

NOW $U = -\vec{P}_m \cdot \vec{B} \ni U =$ ENERGY

AND $(P_m)_z = -g_J\left(\frac{e}{2m}\right) J_z = -g_J\left(\frac{e}{2m}\right) m_J\hbar$

$\therefore U_1 = -p_{m_z} B$

$= g_J\left(\frac{e}{2m}\right)\left(-\frac{3}{2}\right)\hbar B$

$= -\frac{3}{2} g_J\left(\frac{e\hbar}{2m}\right) B$

$= -\frac{3}{2} g_J \beta B \ni \beta = \left(\frac{e\hbar}{2m}\right) =$ BOHR MAGNETRON

F) PARAMAGNETISM (BOLTZMAN DISTRIBUTION)

1) $\bar{U} = \dfrac{\sum U e^{-U/kT}}{\sum e^{-U/kT}}$

$$= \sum_{-J}^{J} m_J g_J \beta B e^{-m_J g_J \beta B/kT} \Big/ \sum_{-J}^{J} m_J g_J \beta B e^{-m_J g_J \beta B/kT}$$

WITH CRANK

$$(\bar{p}_m)_z = g_J \beta J \left\{ \left(\frac{2J+1}{2J}\right) \coth\left[\frac{(2J+1)x}{2J}\right] - \frac{1}{2J}\coth\left(\frac{x}{2J}\right)\right\}$$

$$\ni x = g_J \beta B J/kT$$

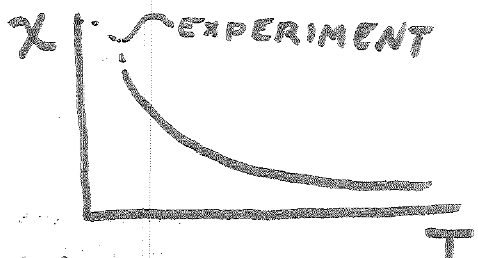
FOR N ATOMS PER UNIT VOLUME

$$\bar{M} = N(\bar{p}_m)_z$$

FOR NORMAL T (NOT TO LOW) AND B (NOT TO HI)

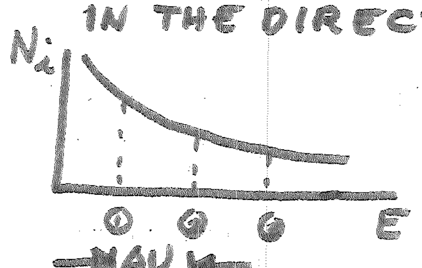
$$M = C'/T \ni C' = N g_J^2 \beta J(J+1)B/2k$$

$$\Rightarrow \chi = M/H = C'/T \quad \text{(CURIES LAW)}$$

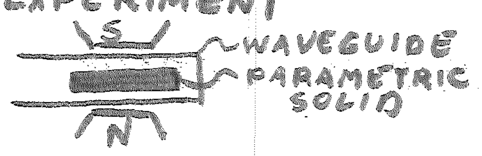


2) THE MAGNETIC MOMENTS AID THE APPLIED FIELD IN PARAMAGNETISM. THE LARGEST NUMBER OF PARTICLES WILL BE WHERE P_z IS LARGEST IN THE DIRECTION OF B_z. (STATE 1)

$$\Delta U = g_J \beta B \ni \beta = e\hbar/2m$$



3) EXPERIMENT



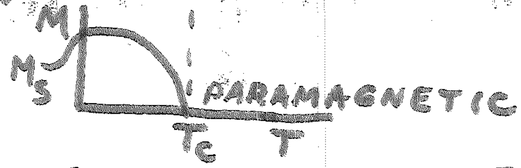
MICROWAVES OF FREQ f.
PHOTONS OF ENERGY $E = hf$.
INCREASING B INCREASES ΔU

AT THE POINT WHERE $g_J \beta B = hf$, THERE WILL BE RESONANT ABSORBTION, AT WHICH POINT g_J MAY BE COMPUTED.

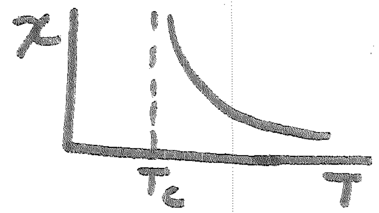
(KNOWN AS ELECTRON PARAMETRIC RESONANCE)

VIII) FERROMAGNETISM
(SPONTANEOUS MAGNETISM WITH NO APPLIED FIELD)

A) M VERY LARGE COMPARED WITH PARAMAGNETIC



SUSCEPTIBILITY OF FERROMAGNETIC



CURIE-WEISS

FERROMAGNETICS: $\chi = \frac{C}{T - T_c}$
PARAMAGNETICS: $\chi = C/T$

B) WEISS

COOPERATIVE EFFECT: MAGNETIC MOMENTS TEND TO LINE UP NEIGHBORING $\vec{p}_m$ IS SAME DIRECTION

$H_{eff} = H + \lambda M$ (λM DUE TO ALIGNMENT)

ABOVE THE CRITICAL T_c, $FERRO_M$ BECOME $PARA_M$

$\chi = M/H_{eff} = C/T$ DUE TO DECREASE OF THE COOPERATIVE EFFECT ABOVE T_c

$\Rightarrow \frac{C}{T} = \frac{M}{H_{eff}} = \frac{M}{H + \lambda M}$

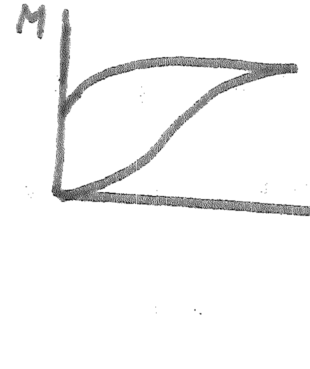
$\Rightarrow M = \frac{C}{T}(H + \lambda M) \Rightarrow \chi = \frac{M}{H} = \frac{C}{T - T_c} \ni T_c = C\lambda$

C) CAUSE OF MAGNETIC MOMENT ALIGNMENT (HYSTERESIS)

- EXCHANGE FORCE CAUSES NEIGHBORING ~~ATOMS~~ SPIN MAGNETIC MOMENTS OF OUTER ELECTRONS IN CERTAIN ATOMS TO BE IN THE SAME DIRECTION -
  - EXAMPLE - THE HYDROGEN MOLECULE -
    TWO POSSIBILITIES
  1. THE ELECTRONS HAVE THE SAME SPIN. EXCLUSION PRINCIPLE TENDS TO FORCE 'EM APART.
     → LOWEST COULOMB POTENTIAL ← ANTI PAR)
  2. THE ELECTRONS HAVE ~~THE SAME SPIN.~~ OPPOSITE SPIN (~~ANTI~~ PARALLEL)

IN $FERRO_M$, THE PARALLEL CONFIGURATION HAS THE LOWEST ENERGY. // SPINS IN ADJ. ATOMS (Fe, Ni, Gd

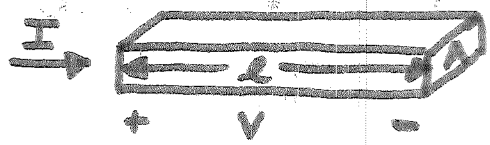
HYSTERESIS

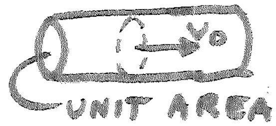


BOUNDRIES WON'T RE-ALIGN EXACTLY AS BEFORE THE FIELD IS APPLIED (LEFT WITH A NET MAGNETIZATION)

IV) FREE ELECTRON THEORY
DEVISED BY DRUDE ~ 1900

A) ~~TRANSIENT ANALYSIS~~ MODEL





V_0 = ELECTRON DRIFT VELOCITY

MOBILITY: $\mu = V_0/E$

CURRENT DENSITY:

$|J| = I/A = |ne^- v_d|$ (UNIT AREA) $\ni n$ = NUMBER OF FREE ELECTRONS

OHM'S LAW:

$V = IR = \frac{\rho l}{A} I$

$E = V/l = \sigma I/A = \rho J \Rightarrow \vec{E} = \rho \vec{J}$ (ANALAGOUS TO $V = IR$)

ρ = RESISTIVITY

$\sigma = 1/\rho$ = CONDUCTIVITY

$\sigma = J/E$

$= nev_0/E$

$= ne\mu$ (μ = MOBILITY)

B) TRANSIENT ALALYSIS

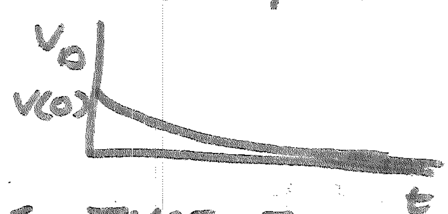
1) OIL DROP IN AIR (?)

$\Sigma F = eE - \left(\frac{m}{\tau}\right) V_D = m \frac{dv_D}{dt}$

2) SUPPOSE E HAS BEEN ON $\rightarrow V_0(0)$

TURN IT OFF

$m \frac{dv_D}{dt} + \frac{m}{\tau} V_0 = 0 \Rightarrow V_0 = V(0) e^{-t/\tau}$



τ IS TIME FOR THE DRIFT VELOCITY TO DROP $1/e$ OF IT'S INITIAL VALUE ($\frac{1}{e}$ OF THE ELECTRONS HAVEN'T COLLIDED AFTER τ SECONDS)

3) WITH FIELD ON

$eE - \frac{m}{\tau} V_0 = m \frac{dv_D}{dt} = 0$

$\Rightarrow eE = \frac{m}{\tau} V_D$

$\therefore \frac{V_D}{E} = e\tau/m = \mu$ (MOBILITY)

AND $\sigma = ne^2\tau/m$

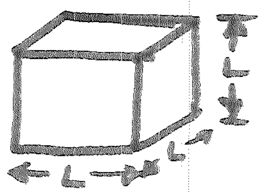
C) SPECIFIC HEAT AT HIGH TEMPERATURES

- FOR FREE ELECTRONS, ∃ 3 NEW DEGREES OF FREEDOM. CLASSICS SAYS

$$C_V = 3R + \underbrace{\tfrac{3}{2}R}_{e^- \text{ K.E.}}$$

NOT SO! THE FREE ELECTRON CONTRIBUTE VERY LITTLE SPECIFIC HEAT TO THE SYSTEM. SOMETHING IS INHIBITING THE ABSORBTION OF THE FREE ELECTRONS. (INHIBITING THE MOMENT ALLIGNMENTS)

E) FREE ELECTRONS IN A METAL



ELECTRONS CONFINED TO A BOX

$U = 0$ INSIDE

$U = \infty$ OUTSIDE

$$\frac{\hbar^2}{2m}\nabla^2\psi + \cancel{U\psi}^{\,0} = E\psi \quad \text{FOR TIME INDEPENDENT } \psi$$

$$\Rightarrow \frac{\delta^2\psi}{\delta x^2} + \frac{\delta^2\psi}{\delta y^2} + \frac{\delta^2\psi}{\delta z^2} + \frac{2m}{\hbar^2}E\psi = 0$$

$$\therefore \psi = C \sin\left(\frac{n_x \pi x}{L}\right)\sin\left(\frac{n_y \pi y}{L}\right)\sin\left(\frac{n_z \pi z}{L}\right)$$

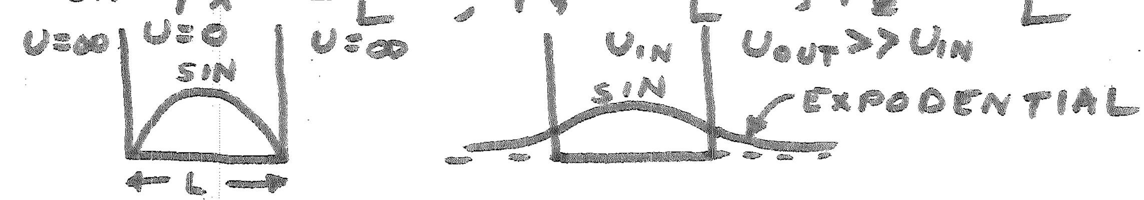
$$-\left(\frac{n_x\pi}{L}\right)^2\psi - \left(\frac{n_y\pi}{L}\right)^2\psi - \left(\frac{n_z\pi}{L}\right)^2\psi = -\frac{2mE}{\hbar^2}\psi$$

$$\Rightarrow \vec{E} = \frac{\hbar^2\pi^2}{2mL^2}\left(n_x^2 + n_y^2 + n_z^2\right)$$

THE e^- MOTION DETERMINED BY $n_x, n_y, n_z \geq 1$

ALSO $\vec{E} = \frac{p^2}{2m} = \frac{p_x^2 + p_y^2 + p_z^2}{2m}$

THEN $p_x = \frac{\hbar \pi x}{L}$; $p_y = \frac{\hbar \pi y}{L}$; $p_z = \frac{\hbar \pi z}{L}$



F) FERMI-DIRAC STATISTICS AND FERMI FUNCTION

1) ASSUMTIONS

a) CAN'T DISTINGUISH ONE ELECTRON FROM ANOTHER (AS OPPOSED TO BOLTZMAN)

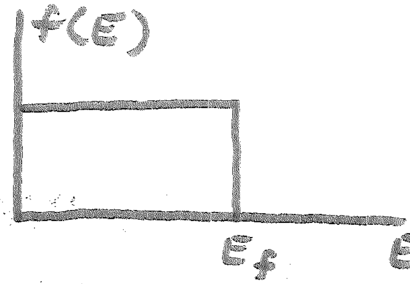
b) EXCLUSION PRINCIPLE

2) FERMI FUNCTION: PROBABILITY THAT THE STATE OF ENERGY E_i IS OCCUPIED BY AN ELECTRON:

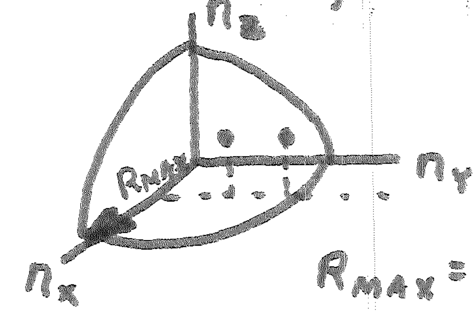
$$f(E_i) = \frac{1}{\exp((E_i - E_f)/kT) + 1} \quad ; \; E_i >> kT$$

E_f = ENERGY OF STATE HAVING 50% CHANCE OF BEING OCCUPIED.

@ $0°K = T$



3) FINDING E_f



CUBIC TYPE LATTICE, EACH POINT REPRESENTING 2 STATES. ALL POINTS INSIDE R_{max} ARE OCCUPIED @ $T = 0°K$

$$R_{MAX} = (n_x^2 + n_y^2 + n_z^2)^{\frac{1}{2}} = \frac{L\sqrt{2mE_{f0}}}{\hbar \pi}$$

OR $R^2_{MAX} = 2mL^2E_{f0}/\hbar^2\pi^2$

THE NUMBER OF OCCUPIED STATES HAVING ENERGY LESS THAN E_{f0}

$$= 2\left[\frac{1}{8}\left(\frac{4}{3}\pi R^3_{MAX}\right)\right]$$

$$= \frac{\pi}{3}\left(2mL^2E_{f0}/\hbar\pi^2\right)^{3/2}$$

FOR N FREE ELECTRONS; $N = \frac{\pi}{3}\left(\frac{2mL^2E_{f0}}{\hbar^2\pi^2}\right)^2$

$$E_{f0} = \frac{\hbar^2}{2m}\left(\frac{3\pi^2 N}{L^3}\right)^{2/3}$$

$$= \frac{\hbar^2}{2m}(3\pi^2 n)^{2/3} \ni n = \text{FREE } e^- \text{ DENSITY}$$

~1 TO 10 ELECTRON VOLTS

G) $g(E)$ AND $N(E)$

1) $g(E)dE$ = NUMBER OF STATES WITH ENERGY TWIXT E AND $E + dE$

$N(E)dE$ = NUMBER OF ELECTRONS WITH ENERGY TWIXT E AND $E + dE$

~~$\Rightarrow f(E)dE$~~

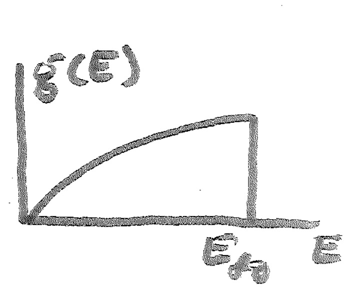
$$\Rightarrow f(E)g(E)dE = N(E)dE$$

2) @ $T = 0°K$, $f(E) = 1$ FOR $0 < E < E_{f0}$
$= 0$ FOR $E > E_{f0}$

$$\Rightarrow \int_0^{E_{f0}} N(E)dE = N = \int_0^{E_{f0}} g(E)dE$$

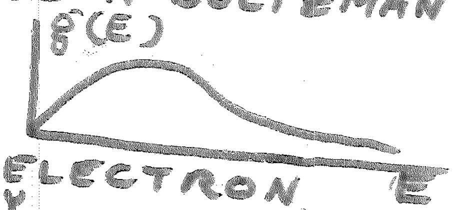
$$N = \frac{L^3}{3\pi^2}\left(\frac{2mE_{f0}}{\hbar^2}\right)^{3/2}$$

$$\Rightarrow g(E) = CE^{1/2} \ni C = \frac{L^3}{2\pi^2}\left(\frac{2m}{\hbar^2}\right):$$



FOR $T>0$:

APPROACHES A BOLTZMAN DISTRIBUTION:



3) AVERAGE ELECTRON ENERGY

a) @ $T=0°K$

$$\bar{E} = \frac{\int_0^{E_{f0}} E N(E)\, dE}{N} \ni N = \frac{2}{3} C E_f^{3/2} = \int_0^{E_f} N(E)\, dE$$

$$\int_0^\infty E N(E)\, dE = \int_0^{E_f} C E^{3/2}\, dE = \frac{2}{5} C E_{f0}^{5/2}$$

$$\Rightarrow \bar{E}_0 = \frac{3}{5} E_{f0}$$

b) $T>0°K$

$$E = \frac{\int_0^\infty E N(E)\, dE}{N} = \int_0^\infty E\, C E^{1/2} f(E)\, dE \Big/ N$$

$$= \frac{\int_0^\infty \frac{C E^{3/2}\, dE}{e^{(E-E_f)/kT}+1}}{N}$$

$$\Rightarrow \bar{E} = \bar{E}(0)\left[1 + \frac{5\pi^2}{12}\left(\frac{kT}{E_{f0}}\right)^2\right]$$

$\therefore$ $\bar{E}$ INCREASES A MIGHT WITH INCREASING T

H) SPECIFIC HEAT

$$U = N\bar{E} = N\bar{E}(0)\left[1 + \frac{5\pi^2}{12}\left(\frac{kT}{E_{f0}}\right)^2\right]$$

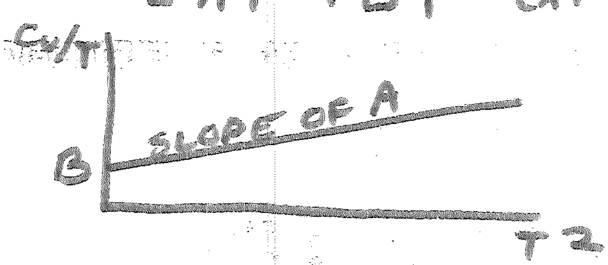
$$C_v = \frac{dU}{dT}\Big|_v = N\bar{E}(0)\frac{5\pi^2}{12}\left(\frac{kT}{E_{f0}}\right)^2$$

FOR 1 MOLE:

$$(C_v)_{ELEC} = RkT\pi^2/2E_{f0} \ll \frac{3}{2}R$$

$$\therefore\ C_v = (C_v)_{VIB} + (C_v)_{ELEC}$$

$$= AT^3 + BT \quad \text{(AT LOW T)}$$

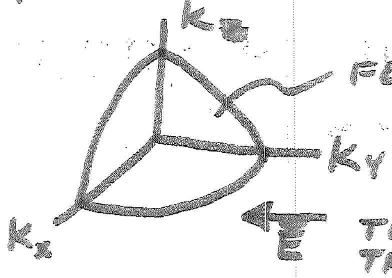


$B = Rk\pi^2/2E_{f0}$

MAY THUS EXPERIMENTALLY COMPUTE E_{f0}

I) K SPACE AND THE FERMI SURFACE

$p = \hbar k$ = ELEC. MOMENTUM



FERMI-SURFACE IN k SPACE

THE APPLIED $\bar{E}$ FIELD WILL SHIFT THE FERMI SURFACE

J) PARAMAGNETISM OF FREE ELECTRON

$$|p_m| = g\left(\frac{e}{2m}\right)\vec{s}$$

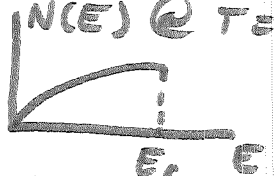
$$(p_m)_z = g\left(\frac{e}{2m}\right)S_z \ni S_z = \pm\frac{1}{2}\hbar \text{ AND } g \simeq 2$$

$$\Rightarrow (p_m)_z = \pm\left(\frac{e\hbar}{2m}\right)$$

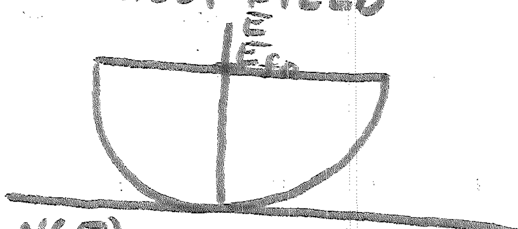
$$U = \vec{p}_m \cdot \vec{B} = -(p_m)_z B \quad \text{(LOW ENERGY)}$$

K) DETERMINATION OF SUSCEPTIBILITY @ T=0°K

N(E) @ T=0°



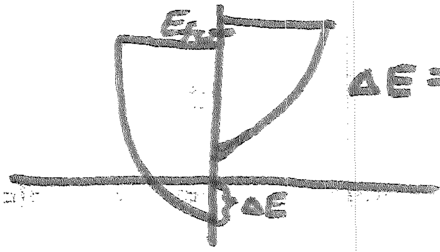
WITHOUT FIELD



N(E) PARALLEL

N(E) ANTI PARALLEL

WITH A FIELD



$$\Delta E = \left(\frac{e\hbar}{2m}\right)B$$

EXCESS PAR. e^- = $N(E_{f_0})\Delta E$

$$N(E)E = \frac{1}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} E_{f_0}^{1/2} p_{m_z} B$$

$\{$ CRANK $\}$

$$\chi = 3n\mu\, p_{mz}^2 / 2E_{f_0}$$

Box
439

(60) C

Name BOB MARKS

Solid State Physics

1. Briefly explain the nature of the following forces between atoms;

(a) covalent forces

COVALENT BONDING RISES WHEN ATOMS SHARE ELECTRONS, THE DIATONIC GASES BEING AN EXAMLE (Cl_2)

nature of force?

6/9

(b) the repulsive force

THE REPULIVE FORCE RISES FROM THE EXCLUSION PRINCIPLE: NO TWO QUANTUM PARTICALS IN A QUANTUM SYSTEM MAY HAVE THE same quantumn numbers (ex: $s = \pm \frac{1}{2}$)

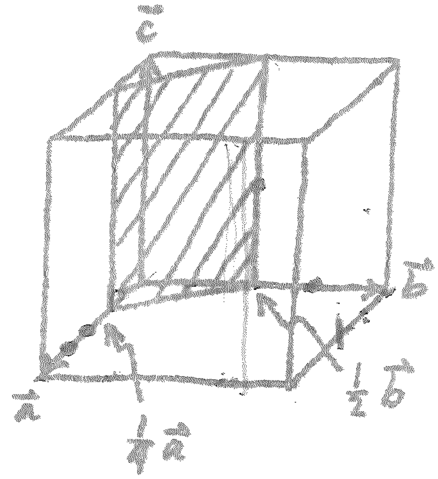
9/9

2. Is a crystal held together by Van der Waal's forces likely to have a higher or lower melting point than an ionic crystal? Why? THE Van der Wall's crystal would have the lower melting point, in that Van der Waalss force acts effectively? only on materials ~~having~~ which solidify near 0° K

weak force

5 /9

3. Given a powder whose crystallites are known to have a primitive cubic structure with lattice constant $a = 2.0\ \text{Å}$



(a) Determine the Miller indices of all planes parallel to the one shown

PLANE WILL INTERSECT @ $\frac{\vec{a}}{h}, \frac{\vec{b}}{k}, \frac{\vec{c}}{l}$

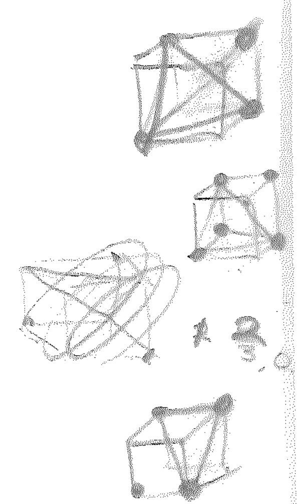
$\Rightarrow \frac{1}{4h}, \frac{1}{2k}, \infty$

$4h, 2k, 0 \Rightarrow (2\ 1\ 0)$

$(\frac{1}{2}, \frac{3}{4}, 0) \Rightarrow (3, 2, 0)$? what is this?

$(\frac{1}{4}\ \frac{2}{3}$

4/9



(b) If this polycrystalline solid is irradiated at various angles θ with x-rays of wavelength $\lambda = 1.0\ \text{Å}$, what are the values of $\sin\theta$ for the first 4 diffraction peaks (starting at $\theta = 0$), and what lattice planes (give indices) give rise to each peak?

$2d \sin\theta = n\lambda$ (BRAGGS LAW)

$\sin\theta = \frac{n\lambda}{2d}$

$\sin\theta = \frac{n\lambda}{2\sqrt{2}}$

FOR RECT $d = \frac{a}{\sqrt{h^2+k^2+l^2}}$

$d = \frac{a}{\sqrt{2}}$?

for all planes?

2/14

4. The expression for the total potential energy of an ionic crystal containing 2N ions was:

$$E = N\left(-\frac{\alpha e^2}{4\pi\epsilon_0 R} + \frac{A}{R^n}\right) \qquad (1)$$

which at absolute zero (0°K) becomes

$$E = -\frac{N\alpha e^2}{4\pi\epsilon_0 R_e}\left(1-\frac{1}{n}\right) \qquad (2)$$

Born has suggested that the second term A/R^n in equation (1), representing the repulsive force between neighboring atoms, should be replaced by $A e^{-R/n}$. Derive the corresponding new equation (2).

$$E = N\left(-\frac{\alpha e^2}{4\pi\epsilon_0}R^{-1} + Ae^{-R/n}\right)$$

$$\left.\frac{\delta E}{\delta R}\right|_{R=R_e} = 0 = N\left(\frac{\alpha e^2}{4\pi\epsilon_0 R^2} - \frac{A}{n}e^{-R/n}\right) \quad ; T = 0°K$$

$$\frac{\alpha e^2}{4\pi\epsilon_0}R^{-2} = \frac{A}{n}e^{-R/n}$$

$$\cancel{\ln\frac{\alpha e^2 n}{4\pi\epsilon_0 A} - 2\ln R_e = 0 \; R/n}$$

$$\Rightarrow A = \frac{n\alpha e^2}{4\pi\epsilon_0 R^2}e^{R_e/n}$$

$$\therefore E = N\left(\frac{-\alpha e^2}{4\pi\epsilon_0 R} + \frac{n\alpha e^2}{4\pi\epsilon_0 R^2}e^{R_e/n}e^{-R_e/n}\right)$$

$$= \frac{N\alpha e^2}{4\pi\epsilon_0 R}\left(\frac{ne^{R/n}}{R} - 1\right)$$

13/17

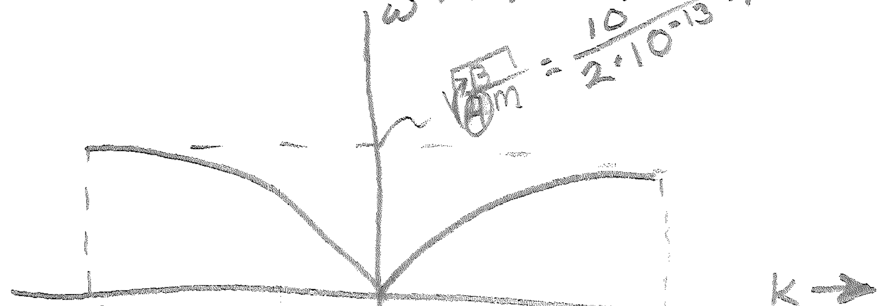
5. Suppose a solid contains a line of atoms .01 meters long with the end atoms fixed, and suppose the mass of the atoms $M = 10^{-26}$ kg, the spacing between atoms $a = 4\times10^{-10}$ meters, and the force constant between neighboring atoms is $\beta = 10^{-10}$ nt/meter.

(a) Draw a figure showing the relationship between the frequency of waves traveling along this line of atoms and the wavelength of these waves (graph of $\omega = 2\pi f$ versus $k = 2\pi/\lambda$).

$\left(\frac{ka}{2}\right)\left(\frac{2\pi}{a}\right)$ $k = \frac{2\pi}{\lambda}$

ω

$\sqrt{\frac{4\beta}{m}} = \frac{10^{-5}}{2\cdot10^{-13}} = .5\times10^{8}\ \frac{\text{RAD}}{\text{SEC}}$



K →

$\cancel{2}\pi/a$

$\frac{\cancel{2}\pi}{a} = 2\pi(100) = 200\pi\ \frac{\text{RAD}}{m}$

7/9

(b) Do higher or lower frequency waves travel faster?

$|V_g| = \left|\frac{\delta\omega}{\delta K}\right| = \frac{a}{2}\sqrt{\frac{\beta}{m}}\cos\frac{ka}{2}\Big|_{-\frac{2\pi}{a}<k<\frac{2\pi}{a}}$ 7/7

$\frac{\delta\omega}{\delta K}$ $\frac{K}{\omega}$

$V_{g\,MAX}$ IS @ K=0 ⇒ FASTER @ LOWER FREQUENCIES

(c) What are the frequencies f of the lowest frequency and highest frequency standing waves for this line of atoms?

FOR STANDING WAVE: $\sin kl = 0$

$\Rightarrow kl = \pi, 2\pi, \ldots, (n-1)\pi$

$\Rightarrow k = \frac{\pi}{l}, \frac{2\pi}{l}, \ldots, \frac{(n-1)\pi}{l}$

$\omega = \sqrt{\frac{4\beta}{m}}\ \sin\frac{(n-1)\pi a}{2l}$

LOWEST f @ n=2 ⇒ $k = \pi/l$

7/17

BOB MARKS

Solid State Physics - Test II

68 C+

I. In the Einstein model of a solid, from which he calculated an expression for the specific heat of an insulator:

A. What assumptions are built into this model?

1) THE ATOMS VIBRATE AT A SINGLE FREQUENCY ✓
2) ASSUMPTION OF BOLTZMAN DISTRIBUTION ✓
3) EACH ATOM ACTED AS 3 MUTUALLY PERPENDICULAR OSCILLATORS ✓
(ie N ATOMS ⇒ 3N OSCILLATORS)

11/11

B. What are the vibration energies allowed the oscillating atoms.

$$E_i = (n + \tfrac{1}{2}) hf ; \; n = 0, 1, 2, 3, \ldots$$

6/6

C. Set up an expression for the average oscillation energy of vibrating atoms

$$\cancel{E = \frac{hf}{e^{hf/kT} - 1}}$$

$$E = \frac{\sum_{i=0}^{\infty} E_i e^{-E_i/kT}}{\sum_{i=0}^{\infty} e_i^{-E_i/kT}}$$

10/10

D. Outline, without all the mathematical details, the procedure for determining an expression for the specific heat C_V from the average vibrational energy.

① SUBSTITUTE E_i INTO $\overline{E}$ EXPRESSION

② CANCEL EXPODENDENTIALS FOUND? IN BOTH NUM. AND DEN.

③ LET $X = hf/KT$

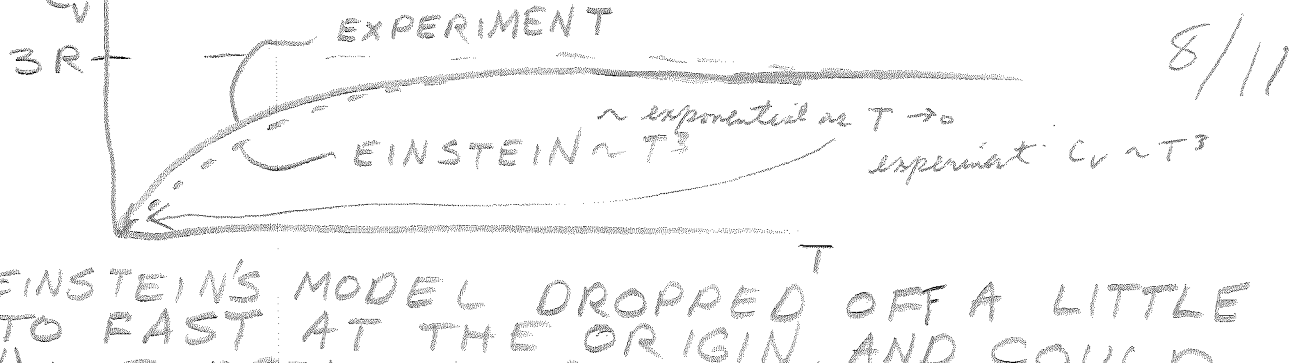
④ EXPAND NUM. AND DEN., NOTICING DENOMENATOR $= \left(\frac{1}{1-e^{x}}\right)$?, AND THAT THE NUMERATOR IS IT'S DERIVITIVE, AND SUBSTITUTE IN INTEGRAL

⑤ $U = 3N\overline{E}$, SO MULTIPLY $\overline{E}$ BY 3N TO OBTAIN U. EVALUATE INTEGRAL.

⑥ $C_V = \left.\frac{\delta U}{\delta T}\right|_V$

8/8

E. How did Einstein's C_V compare with the experiment at low temperatures, and what might be done to get better agreement?



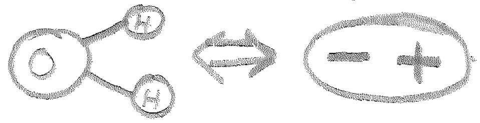
8/11

EINSTEIN'S MODEL DROPPED OFF A LITTLE TO FAST AT THE ORIGIN, AND COULD HAVE BEEN INPROVED BY CONSIDERING MORE THAN JUST A SINGLE FREQ (AS DID DEBYE). HE MIGHT HAVE TRIED OTHER DISTRIBUTIONS. ALSO, SOME OF THE PARAMETERS TAKEN OUTSIDE THE INTEGRAL SIGN IN THE DERIVATION WEREN'T INDEP OF THE VARIABLE OF.

II. Polarization of a Dielectric

A. Describe the three kinds of polarization processes which occur in dielectrics and cause a reduction in the electric field

1) ORIENTATIONAL – DUE TO THE GEOMETRY OF A MOLECULE, IT IS LOPSIDED IN THE SENSE OF CHARGE, SUCH AS WATER:



electric fields partially orient these permanent dipoles in $\vec{E}$ direction

ONIC

2) ELECTRIC – DUE TO NON-SYMMETRIC ROTATION OF ELECTRONS ABOUT THEIR NUCLEUS.

10/15

3) IONIC – RISES FROM ATTRACTION OF IONS. EX: Na^+Cl^-

?

Shift of ions due to applied field

B. Given a dielectric which has a cubic lattice structure of one type of atom only, Starting with the general relationship between the dielectric constant κ and polarization P, and the equation relating the local field at the position of an atom to the macroscopic field E in this dielectric, derive the expression relating its dielectric constant to the electronic polarizability of the atom (Clausius – Mosotti equation).

$$\vec{D} = \epsilon_0 \vec{E} + \vec{P} = K\epsilon_0 E \Rightarrow K = \frac{\epsilon_0 E + \vec{P}}{\epsilon_0 E} = 1 + \frac{P}{\epsilon_0 E}$$ ✓

$$E_{LOC} = \underbrace{E_1 + E_2}_{E} + E_3 + \cancel{E_4} \; 0 \text{ (CUBIC)}$$

$$= E + E_3$$

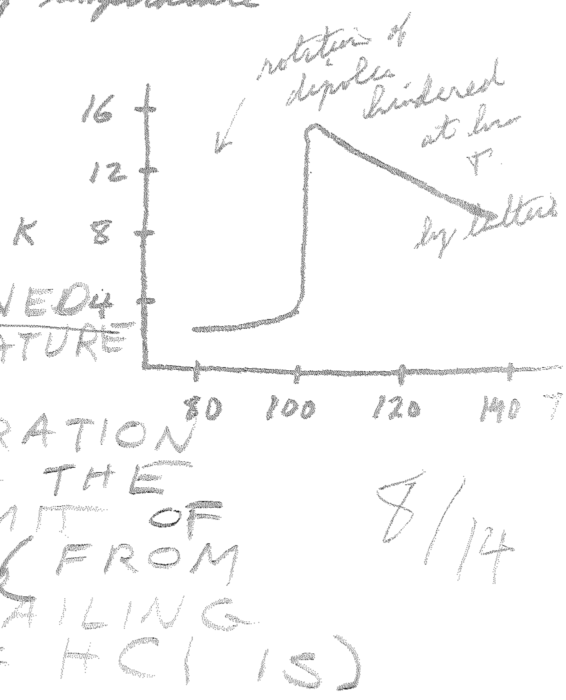
$$E_3 = \frac{P}{3\epsilon_0}$$

7/25

$$\alpha = \frac{P}{E_{Loc}}$$ ✓

$$\frac{P}{E_{Loc}}$$

c. Explain briefly the following graph showing the dielectric constant of solid HCl as a function of temperature (i.e. why the sudden change at ~100°K and why the decrease at higher T?)



FOR SOME REASON, DIPOLES SUDDENLY BECOME ALLIGNED AT 100° AND AS TEMPERATURE INCREASES, MOLECULAR AND THUS DIPOLE VIBRATION INCREASES, DECLINING THE DIPOLES TO THE LIMIT OF RANDOMNESS AGAIN (FROM WHATEVER THE PREVAILING POLARIZABILITY OF HCl IS)

8/14

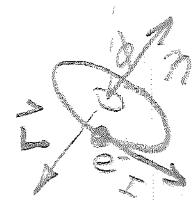
Name BOB MARKS

Solid State Physics – Test III

77 B

I. Magnetism in Solids (Insulators)

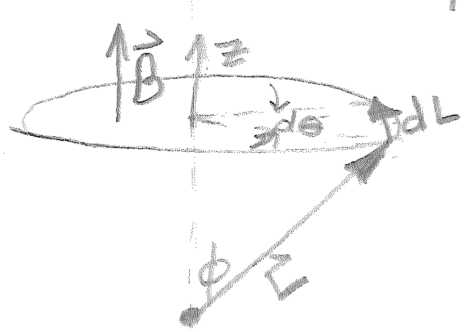
A. An electron in orbit about a nucleus has an angular momentum $\vec{l}$ causing a magnetic moment $\vec{p}_m = -(\frac{e}{2m})\vec{l}$. Show that the application of a magnetic field $\vec{B}$ making angle ϕ with the direction of $\vec{l}$ causes the orbit to precess about the direction of $\vec{B}$ with angular frequency $\vec{\omega}_L = (\frac{e}{2m})\vec{B}$ (rad/sec.)



$$p_m = -\left(\frac{e}{2m}\right) l$$

$$\tau = \vec{p}_m \times \vec{B} = \frac{d\vec{L}}{dt}$$

18/20



LET $\omega_L = -d\theta/dt$

NOW $d\vec{L} = |p_m \times \vec{B}|\,dt$

$$= p_m \sin\phi\, B\, dt$$

$dL = \cancel{\quad} (L \sin\phi)\, d\theta$

$$p_m \cancel{\sin\phi} B\, dt = L \cancel{\sin\phi}\, d\theta$$

$$\omega_L = \frac{d\theta}{dt} = \frac{-p_m B}{L} = \frac{(\frac{e}{2m}) L B}{L} = \frac{e}{2m}\vec{B}$$

a lot of sign difficulty

8. Suppose that some of the atoms in a particular solid have magnetic moments. Explain briefly how it happens that these atoms will contribute a paramagnetic effect when a magnetic field is applied to the solid.

THERE WILL BE AN ADDITIONAL ~~AND~~ ORBITAL ~~OR~~ ANGULAR MOMENTUM INDUCED IN THE SYSTEM, ~~[illegible]~~ ~~ANGULAR MOMENTUM~~

$$\vec{p}_m = \left(\frac{-e}{2m}\right)\vec{L}_{eff} \ni \vec{L} = [L(L+1)]^{1/2}\hbar$$

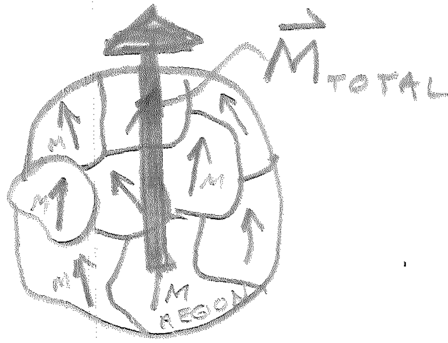
$$\vec{B} = \mu_0\vec{H} + \underbrace{\lambda\vec{M}}_{\text{DUE TO } L_{eff}}$$

4

c. What is the source or cause of the spontaneous magnetiz. in a ferromagnetic solid, without any applied field?

~~THE~~ SPONTANEOUS MAGNETIZATION IS A RESULT OF COOPERATIVE ALIGNMENT OF ADJACENT DIPOLES. EACH GROUP OF COOPERATIVELY ALIGNED DIPOLE CONSTITUTES A REGION OF NET MAGNETIZATION, EACH ADJACENT REGION COOPERATIVELY ALIGNS (SOMEWHAT), CAUSING A NET MAGNETIZATION, M. (IN PRESENCE OF B FIELD)

electron spin magnetic moment



what causes alignment of spin moments in neighboring atoms

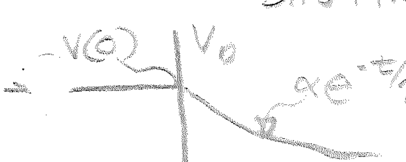
8/14

II, Free Electron Theory of Metals

A. What is the meaning of the letter τ in the expression for the electrical conductivity $\sigma = \frac{ne^2\tau}{m}$ and what effect does changing the temperature have on it?

10/10

τ IS THE TIME (IN TRANSIENT ANALYSIS) FOR INITIAL average DRIFT VELOCITY TO REDUCE BY A FACTOR OF 1/e. (IN THE CASE OF SHUTING OFF AN ESTABLISHED FIELD) FOR 1/e TH OF THE e⁻ TO BUMP INTO SOMETHING

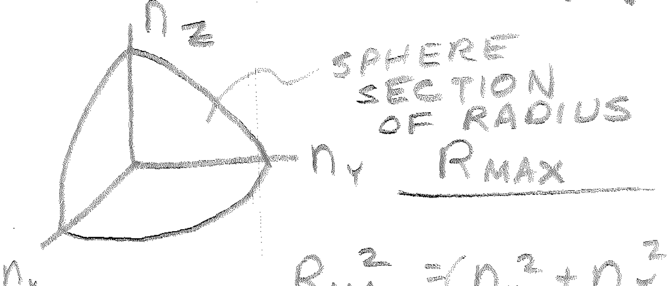


THE HIGHER THE TEMPERATURE THE LARGER V_D, (THE ELECTRONS MOVE FASTER) AND THUS THE GREATER CHANCE FOR COLLISION, ERGO, THE SMALLER τ ✓

B. Given the expression for the energies allowed a free electron in a metal cube, $E = \left(\frac{\hbar^2\pi^2}{2mL^2}\right)(n_x^2 + n_y^2 + n_z^2)$, show that the Fermi energy at $T = 0°K$ is related to the number N of free electrons per unit volume L^3 by:

$$\frac{N}{L^3} = \frac{\pi}{3}\left(\frac{2mE_{F0}}{\hbar^2\pi^2}\right)^{3/2}$$

L S M



$$R_{MAX}^2 = (n_x^2 + n_Y^2 + n_z^2)_{MAX} = \frac{2mL^2E_{F0}}{\hbar^2\pi^2}$$

EACH POINT REPRESENTS 2 STATES.

$$\Rightarrow N = \frac{1}{8}\left[2\left(\frac{4}{3}\pi R_{MAX}^3\right)\right]$$

$$= \frac{\pi}{3}R_{MAX}^3$$

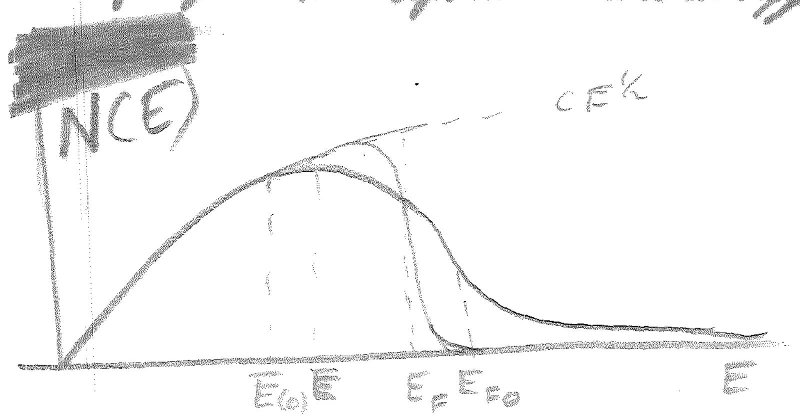
$$= \frac{\pi}{3}\left(\frac{2mL^2E_{F0}}{\hbar^2\pi^2}\right)^{3/2}$$

20/20

$$= \frac{\pi}{3}L^3\left(\frac{2mE_{F0}}{\hbar^2\pi^2}\right)^{3/2}$$

$$\therefore \frac{N}{L^3} = \frac{\pi}{3}\left(\frac{2mE_{F0}}{\hbar^2\pi^2}\right)^{3/2}$$

Draw a graph showing the approximate energy distribution of free electrons in a solid at room temperature (i.e. show how the number of electrons in an energy interval of size dE depends on the energy E).



5/7

$f(E)\, g(E)\, dE = N(E)\, dE$

(1) Mark the "Fermi energy" on this graph and explain what is meant by the term "Fermi energy".

THE FERMI ENERGY (E_f) IS THE ENERGY AT WHICH THE PROBABILITY OF OCCUPANCY OF AN ENERGY LEVEL BY AN ELECTRON IS 50%

7/7

(2) Given two energy intervals dE at low energies E_1 and E_2 where $E_2 = 2E_1$. What is the ratio of the number of particles in the higher energy interval to that in the lower?

FOR LOW ENERGYES: $\frac{C\sqrt{E_2}}{C\sqrt{E_1}} = \frac{\sqrt{2E_1}}{\sqrt{E_1}} = \boxed{\sqrt{2}}$

8/8

1

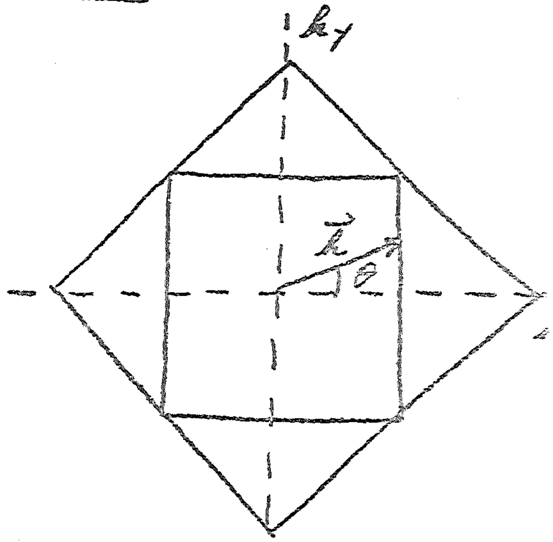
(45)

C

Name BOB MARKS (BOX 439)

Solid State Physics – Test IV

① The figure shows the first two Brillouin zones for electron wave $\vec{k}$ vectors in a cubic lattice (unit cell cube edge a)



(a) What is likely to happen to an electron having a propagation wave vector $\vec{k}$ as shown? Justify your answer mathematically. (14)

(DIFFRACTED)

BRAGG'S LAW YIELDS

$\lambda = 2a\sin\theta$ (FOR CONSTRUCTIVE INTERFERENCE)

$k = \frac{2\pi}{\lambda}$

$\frac{2\pi}{k} = 2a\sin\theta \Rightarrow k = \frac{2\pi}{2a\sin\theta}$

so?

12

35.5

236.5
59.5

(b) Suppose that this crystal has the same number of electrons as it has electron states per band. What determines whether it will be a metal, insulator, or semiconductor? (13)

WHICH OF THE BANDS SECTIONS GETS FILLED FIRST

HIGHER ENERGY

METAL →

INSUL →

7

? explain

$$\vec{D} = \epsilon_0 \vec{E} + \vec{P} = K\epsilon_0 E \Rightarrow K = \frac{\epsilon_0 E + \bar{P}}{\epsilon_0 E} = 1 + \frac{P}{\epsilon_0 E}$$

$$E_{Loc} = \underbrace{E_1 + E_2}_{E} + E_3 + \cancel{E_4} \rightarrow 0 \text{ (CUBIC)}$$

$$= E + E_3$$

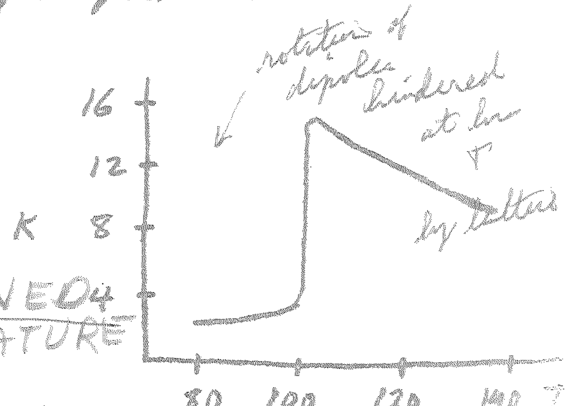
$$E_3 = \frac{P}{3\epsilon_0}$$

7/25

$$\alpha = \frac{P}{E_{Loc}}$$

$$\frac{P}{E_{Loc}}$$

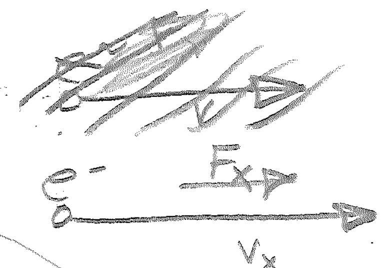
c. Explain briefly the following graph showing the dielectric constant of solid HCl as a function of temperature (i.e. why the sudden change at ~100°K and why the decrease at higher T?)

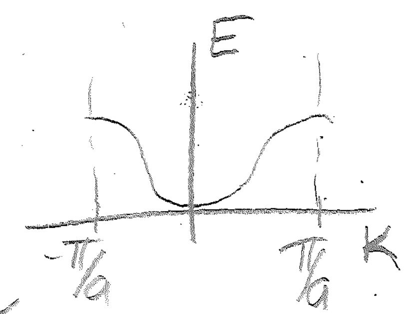


FOR SOME REASON, DIPOLES SUDDENLY BECOME ALLIGNED4 AT 100° AND AS TEMPERATURE INCREASES, MOLECULAR AND THUS DIPOLE VIBRATION INCREASES, DECLINING THE DIPOLES TO THE LIMIT OF RANDOMNESS AGAIN (FROM WHATEVER THE PREVAILING POLARIZABILITY OF HCl IS)

8/14

② An electron is moving in the x direction in a periodic lattice and is being acted upon by an electric force $\vec{F}$. Derive an expression for its acceleration as a function of $\vec{F}$ and the E vs. k curve for motion along this axis (assuming force $\vec{F}$ is along the x axis). (22)





10

$v = \frac{d\omega}{dK}$

$a = \frac{dv}{dt} = \frac{d^2\omega}{\delta K\, \delta t}$ ⟵ method ⟶

$E = hf$
$= \hbar\omega$
$dE = \hbar d\omega$
$d^2E = \hbar d^2\omega$

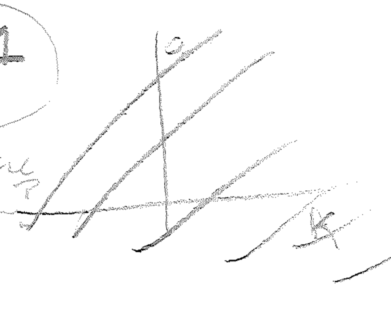
$F_x = m^* a \Rightarrow a = \frac{F_x}{m^*} = \cancel{\frac{F dx}{m^*}}$

$\cancel{dF_x = F dx}$

$\cancel{a = d^2E}$

$m^* = \frac{1}{\hbar}\left(\frac{\delta^2 E}{\delta k^2}\right)^{-1}$

⟵ where from?

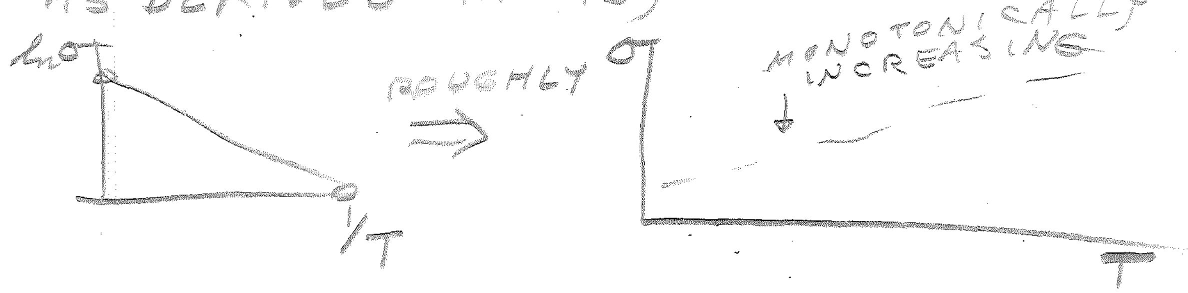


$F_x = m^* a$

$a = \frac{F_x}{m^*} = \frac{F_x \hbar^2 \frac{\delta^2 E}{\delta k^2}}{}$

③ The conductivity of an intrinsic semiconductor increases with temperature while that of a metal decreases. Explain (13)

THE INCREASE IN CONDUCTIVITY OF AN INTRINSIC SEMI CONDUCTOR AS DERIVED IN 4b)



Explain?

④ From the expressions $n = N_c e^{-(E_c - E_F)/kT}$ for the number of electrons per unit volume in the conduction band, and $p = N_v e^{-(E_F - E_v)/kT}$ for the number of holes per unit volume in the valence band: (22)

(a) derive an equation relating the conductivity of an intrinsic semiconductor to the energy gap and temperature (among other things). $n = p$

$$n = N_c e^{-(E_c - E_f)/kT} \; ; \; p = N_v e^{-(E_f - E_v)/kT}$$

$$\sigma = n e \mu_n + p e \mu_p$$

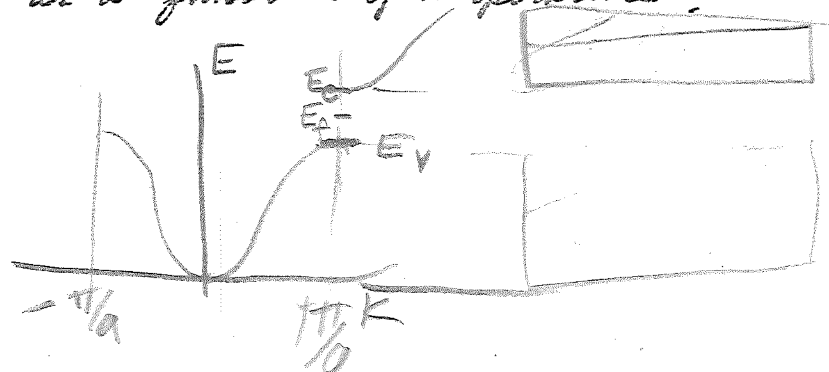
$$\cancel{= (N_c e \mu_n + N_v \mu_p e) e^{-(E_c - E_f)/kT}}$$

$$\cancel{= (N_c \mu_n + N_v \mu_p) e \, e^{-(E_c - E_f)/kT}}$$

BACK OF PREVIOUS PAGE

$$= e \left(N_c \mu_n e^{-(E_c - E_f)/kT} + N_v \mu_v e^{-(E_f - E_v)/kT} \right)$$

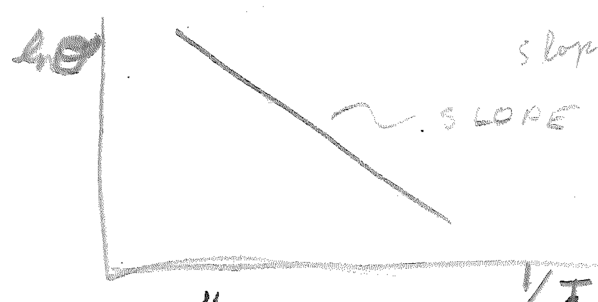
(b) Briefly explain how the result of part (a) allows one to measure the energy gap by measuring conductivity as a function of temperature.



8

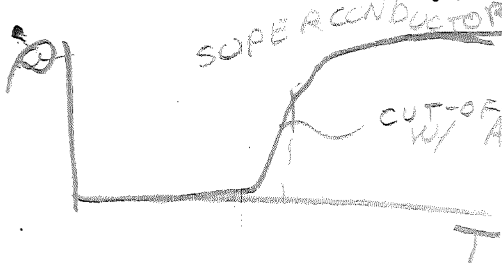
~~DERIVED EQUATION (WHICH IS WRONG)~~

slope = $-E_g/2k$



SLOPE PROPORTIONAL TO E_g $\left(= \frac{E_g}{2k}\right)$

⑤ What is the "Meissner effect" in superconductors?



SUPERCONDUCTOR

CUT-OFF SHARPENS W/ ADDED IMPURITIES

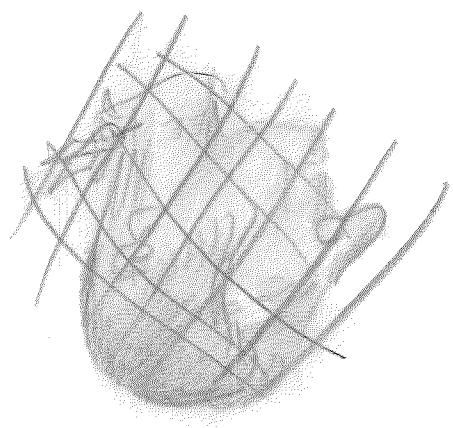
0

TWIN PAIRS

(OPPOSITE S & K)

ALL FILL

b) Derive an expression for the electric field intensity E at any position x along the positive x axis, starting from the expression for V found in part (a). (12)

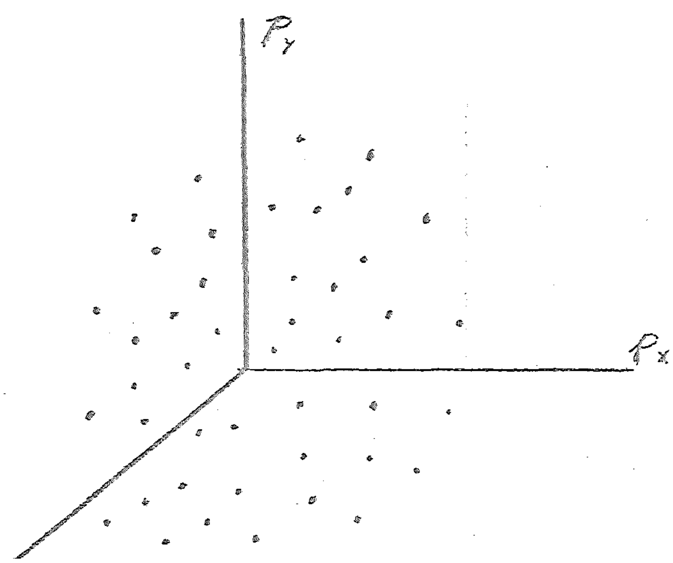


STATISTICAL MECHANICS

Solids, like gases, are made up of large numbers of interacting particles. In the absence of any information about individual particles one can still predict with accuracy many properties of such an assembly, using the laws of probability and statistics. One of the central problems of statistical mechanics is concerned with the prediction of the most probable energy distribution of a large number of interacting particles. This distribution, called the "equilibrium" distribution, has been found to have such a high probability of occurence when the number of particles is large, that significant deviations from this distribution are very unlikely (but not impossible).

The energy E of an individual particle is the sum of its kinetic energy and its potential energy. The kinetic energy depends only on the particle's momentum and the potential energy only on its position so that its energy is completely specified by six quantities, three momentum components (e.g. p_x p_y, p_z) and three position coordinates (e.g. x,y,z). At any instant, each particle of the assembly will have six values associated with it, one for each of the quantities mentioned above. The task of finding the energy distribution then becomes one of finding the numbers of particles having values between x, y, z, p_x, p_y, p_z and $x + \Delta x$, $y + \Delta y$, $z + \Delta z$, $p_x + \Delta p_x$, $p_y + \Delta p_y$, $p_z + \Delta p_z$.

For example, suppose the particles are free so that the potential energy $U = 0$ for all particles (an ideal gas). In this case the energy of the particle is completely specified by its momentum components; it may be represented by a point in "momentum space" as shown below.



One may think of this momentum space as being divided into "cells" of dimensions Δp_x, Δp_y, Δp_z and then try to find the most probable distribution of points among the cells in order to determine the energy distribution. In general, $U \neq 0$ and the cells are six dimensional cells in a six dimensional "phase space".

Suppose now that one has N particles and wishes to determine the most probable distribtuion of them among cells of energy E_1, E_2, E_3, etc. The probability of a particular distribution is proportional to the number of ways W of making the distribution, and it can be shown that <u>if the particles are distinguishable from each other</u>

$$W = \frac{N!}{N_1!\ N_2!\ N_3! \ldots} \tag{1}$$

where N_1 = number of particles in cell 1, etc.

<u>Example</u>: Suppose there are 4 particles to distribute between 2 cells.

(possibility 1): all 4 in cell 1; only one way to do it

$$W = \frac{4!}{4!\ 0!} = 1$$

(possibility 2): 3 in cell 1, 1 in cell 2; four ways to do it....with particle a, b, c, or d in cell 2

$$W = \frac{4!}{3!\ 1!} = 4$$

(possibility 3): 2 in each cell; six possible combinations .... identify them yourself

$$W = \frac{4!}{2!\ 2!} = 6$$

(possibility 4): 3 in cell 2; similar to possibility 2

(possibility 5): all 4 in cell 2; similar to possibility 1

In this case possibility 3 describes the equilibrium distribution and it is not much more probable than possibilities 2 or 4 (this would not be the case if there were a large number of particles and cells).

In order to obtain a general expression for the equilibrium energy distribution, one maximizes W (equation 1) with respect to variable N_1, N_2,......
(LaGrange's method of undetermined multipliers) with the restrictions

$$N = N_1 + N_2 + N_3 + \ldots\ldots\ldots\ldots\ldots = \sum N_i$$

$$E = N_1 E_1 + N_2 E_2 + \dots\dots\dots = \sum N_i E_i$$

and gets the most probable energy distribution

$$N_i \propto e^{-E_i/kT} \qquad (2)$$

where N_i is the number of particles having energy E_i. This expression is directly useful only where energies are discrete so that a particular energy E_i is associated with each cell. If the energy is continuous the cells must be considered infinitesimal and of volume $d\Omega$ in six dimensional phase space (e.g. in cartesian coordinates $d\Omega = d\,p_x\,d\,p_y\,d\,p_z\,dx\,dy\,dz$). The number of particles per infinitesimal cell is then

$$dN \propto e^{-E/kT}\,d\Omega \qquad (3)$$

Equations (2) and (3) represent the classical Maxwell-Boltzmann equilibrium distribution.

One of the difficulties with the above analysis is that particles can't be labeled a,b,c,.....they are indistinguishable. Thus in the example given concerning the distribution of 4 particles between 2 cells, there are not actually four distinct ways to put three particles in cell 1 and one in cell 2; the expression (1) for W is incorrect. Also, according to quantum mechanics, the position and momentum of a particle can be determined simultaneously only with uncertainty

$$p_x \Delta x > \hbar/2 \qquad \text{etc.}$$

and therefore the cell volume can't be infinitesimal but must be of the order $\hbar^3/8$ or greater to ensure knowledge of when a particle is in a particular cell. When these facts are taken into account, an analysis similar to the above yields for the equilibrium number of particles in a state of energy E_i.

$$N_i \propto \frac{1}{B\,e^{E_i/kT} - 1} \qquad (4)$$

which is the Bose-Einstein distribution function.

In the case of particles having half integral values of spin (e.g. electrons, protons, neutrons) there is also a restriction on the number of particles that can go into a particular state. In a given system, only one particle is allowed to occupy a state having a given set of quantum numbers. One determines the probability $f(E_i)$ that a state of energy E_i is occupied rather than the number of particles in the state. The equilibrium result is

$$f(E_i) = \frac{1}{B\,e^{E_i/kT} + 1} \qquad (5)$$

where the probability function $f\ (E_i)$ is called the Fermi function. The quantity B is not temperature independent and may be written

$$B = e^{-E_F/kT}$$

resulting in

$$f\ (E_i) = \frac{1}{e^{(E_i - E_F)/kT} + 1} \qquad (6)$$

where E_F is called the Fermi energy of the system and is almost, but not quite, temperature independent. The Fermi energy E_F is defined as the energy of that state which has a 50% chance of being occupied by some particle, since when $E_i = E_F$, $f = 1/2$. States having lower energies ($E_i < E_F$) are more likely to be occupied ($f > 1/2$), and states of higher energy ($E_i > E_F$) less likely to be occupied ($f < 1/2$).

(1)

Test next ... (... ...)

I. Assignment: pp. 133 - 35, prob. 2, 3

II. Specific Heat for Solids

A. Einstein

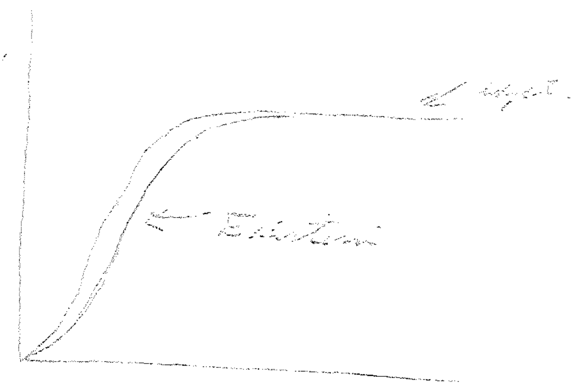
only one vibration frequency for atoms

as $T \to 0$

$C_v \to 0$ as an exponential

$\longrightarrow$ experiment

$C_v \sim T^3$ at low T



B. Debye

(1) 3N different frequencies of vibration — the standing wave frequencies of a continuous medium with fixed surfaces

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} = \frac{1}{v^2}\frac{\partial^2 u}{\partial t^2}$$ cube of edge L

$$u = u_0 \sin\left(\frac{n_x \pi x}{L}\right)\sin\left(\frac{n_y \pi y}{L}\right)\sin\left(\frac{n_z \pi z}{L}\right)\cos 2\pi f t$$

$$n_x, n_y, n_z = 1, 2, \ldots$$

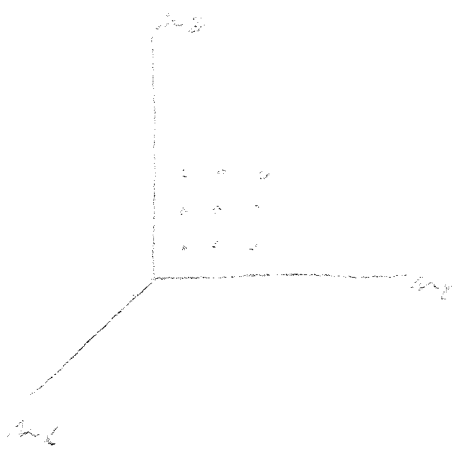
Substitute

$$\left[u_0 \sin\left(\frac{n_x \pi x}{L}\right)\sin(\quad)\sin(\quad)\cos 2\pi f t\right]\left[-\frac{n_x^2\pi^2}{L^2} - \frac{n_y^2\pi^2}{L^2} - \frac{n_z^2\pi^2}{L^2}\right]$$

$$= \left[\qquad\qquad\qquad\qquad\right]\left[-\frac{1}{v^2}4\pi^2 f^2\right]$$

$$\longrightarrow \left(\frac{\pi^2}{L^2}\right)(n_x^2 + n_y^2 + n_z^2) = \frac{4\pi^2 f^2}{v^2}$$ $\longrightarrow$ standing wave

Allowed frequencies $\quad f = \frac{v}{2L}\sqrt{n_x^2 + n_y^2 + n_z^2}$



- Plot allowable modes in "n-space"
  - each n_x, n_y, n_z integer
    to a particular oscillation mode

Let $R^2 = n_x^2 + n_y^2 + n_z^2 = \frac{4L^2 f^2}{v^2}$

$R = \frac{2Lf}{v}$ = distance from origin to any point

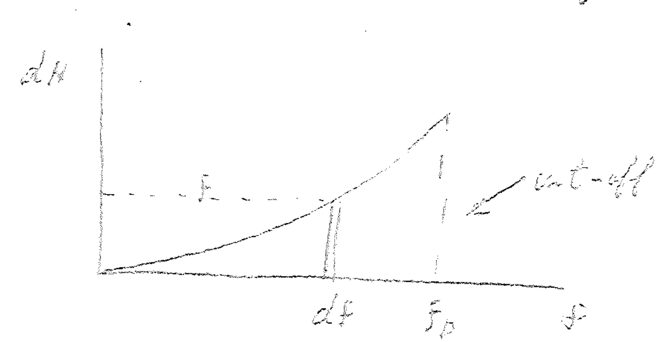
$dR = \frac{2L}{v}\, df$

— integer space for enumeration of modes
→ 1 mode per unit volume

— between R and $R + dR$, volume $= \frac{1}{8}(4\pi R^2\, dR) = \frac{\pi}{2} R^2\, dR$

No. of modes between corresponding frequencies f and $f + df$

$$dN = \frac{\pi}{2}\left(\frac{4L^2 f^2}{v^2}\right)\left(\frac{2L}{v}\, df\right) = \frac{4\pi L^3}{v^3} f^2\, df = \frac{4\pi V}{v^3} f^2\, df$$



Actually there are two transverse and one longitudinal mode for each point in n space — T and L waves have different speeds

$$\boxed{dN = 4\pi V\left(\frac{2}{v_t^3} + \frac{1}{v_l^3}\right) f^2\, df}$$

Cut-off frequency such that

$$\int_0^{f_D} dN = 3N$$

$$4\pi V\left(\frac{2}{v_t^3}+\frac{1}{v_l^3}\right)\int_0^{f_D} f^2\,df = 3N \qquad \left\{\begin{matrix}\text{assume } v_t,\ v_l \\ \text{independent of } f\end{matrix}\right\}$$

integrate, solve for f_D $\longrightarrow$ $f_D = \left\{\frac{3}{4\pi}\frac{N}{V}\left[\frac{2}{v_t^3}+\frac{1}{v_l^3}\right]^{-1}\right\}^{1/3}$

For a given f $\quad E = \frac{hf}{e^{hf/kT}-1}$ $\quad$ (assume same as Einstein's E)

$$U = \int_0^{f_D} E\,dN = \int_0^{f_D}\left(\frac{hf}{e^{hf/kT}-1}\right)dN = 4\pi V\left(\frac{2}{v_t^3}+\frac{1}{v_l^3}\right)\int_0^{f_D}\frac{hf^3\,df}{e^{hf/kT}-1}$$

If $x = \frac{hf}{kT}$ and $x_D = \frac{hf_D}{kT}$

$$U = 9N\left(\frac{kT}{hf_D}\right)^3 kT\int_0^{x_D}\frac{x^3\,dx}{e^x-1}$$

<u>High T</u> $\quad U \simeq 9N\left(\frac{kT}{hf_D}\right)^3 kT\int_0^{x_D}\frac{x^3\,dx}{x}$

since $e^x = 1 + \frac{x}{1!} + \frac{x^2}{2!} + \frac{x^3}{3!}$ and $x \ll 1$ over whole range

$$U = 9N\left(\frac{kT}{hf_D}\right)^3 kT\left(\frac{1}{3}\frac{h^3 f_D^3}{k^3T^3}\right) = 3NkT$$

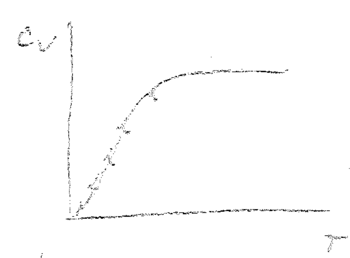
$$\boxed{C_v = \frac{\partial U}{\partial T}\Big]_V = 3N_0 k = 3R}$$

<u>Low T</u> $\quad U \simeq 9N\left(\frac{kT}{hf_D}\right)^3 kT\left[\int_0^{\infty}\frac{x^3\,dx}{e^x-1} = \frac{\pi^4}{15}\right]$

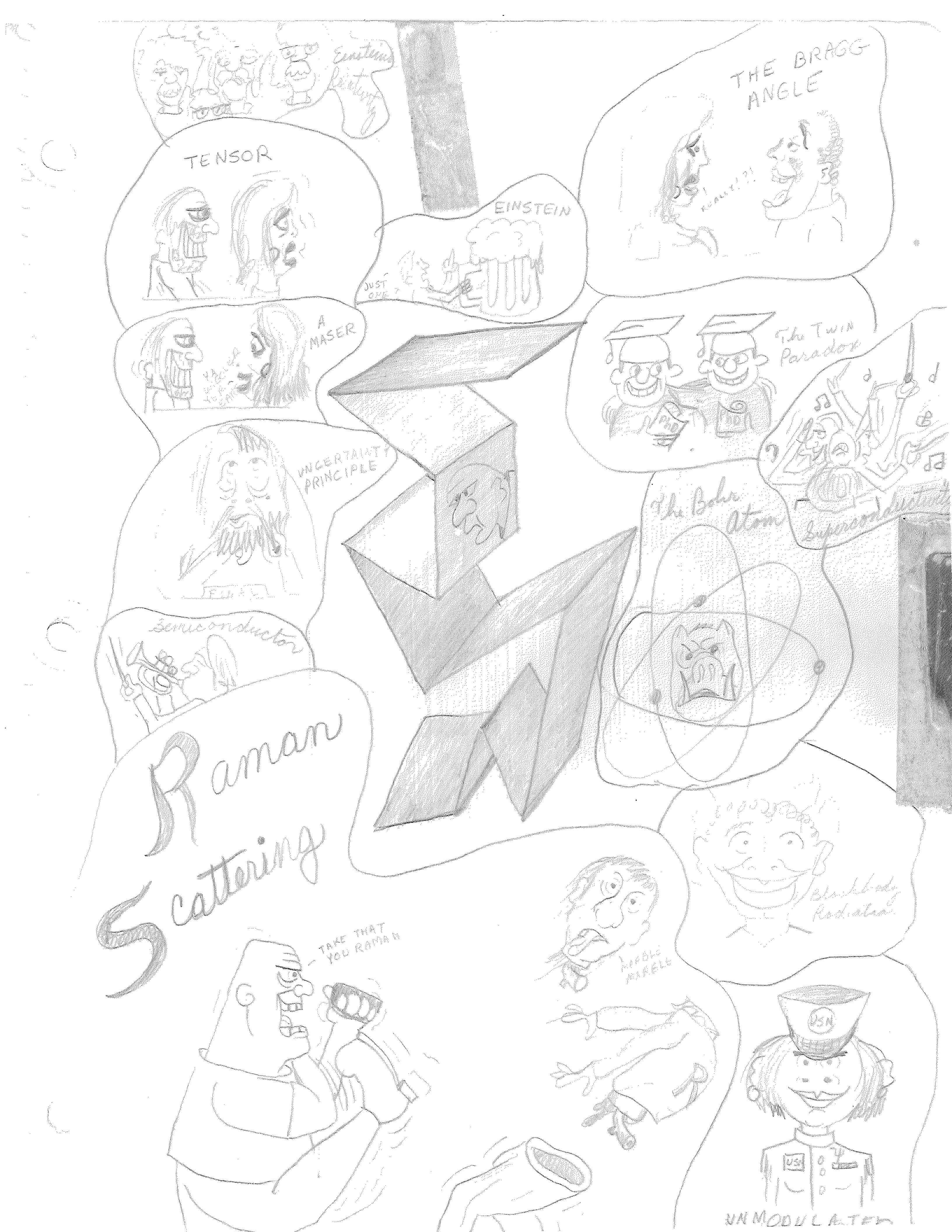
$$U = \frac{3}{5}\pi^4 NkT\left(\frac{T}{\theta_D}\right)^3 \text{ where } \boxed{\theta_D = \frac{hf_D}{k}} = \text{Debye Temp.}$$

$$C_v = \frac{\partial U}{\partial T}\Big]_V = \frac{12}{5}\pi^4 R\left(\frac{T^3}{\theta_D^3}\right)$$

$C_v \to 0$ as T^3



in very good agreement with experiment even though we know we have only approximated the actual frequency distribution and have assumed that all waves travel at same speed


Einstein's Lottery
TENSOR
EINSTEIN
JUST ONE
THE BRAGG ANGLE
A MASER
The Twin Paradox
UNCERTAINTY PRINCIPLE
Superconductivity
The Bohr Atom
Semiconductor
Raman Scattering
Black-body Radiation
TAKE THAT YOU RAMAN
MARBLE MARELL
UNMODULATED

EE 53.3
DUE 9-17-75

BOB MARKS

1.4. $\lambda = 2500\text{Å}$, $V_0 = 3.06\,V$

WORK FUNCTION: $\mathcal{E}_w = \mathcal{E}_b - \mathcal{E}_f$

$\mathcal{E}_b$ = ENERGY OF LIGHT = $h\nu = \frac{hc}{\lambda}$

$\mathcal{E}_f$ = ENERGY OF ELECTRONS = eV_0

$$\mathcal{E}_b = \frac{1.24 \times 10^4\ eV\text{-Å}}{2500\text{Å}} = 4.96\ eV$$

$$\mathcal{E}_f = (1.602 \times 10^{-19}\ \text{coul})(3.06V) \times \frac{1\ \text{joule}}{1\ \text{coul-V}} \times \frac{6.242 \times 10^{18}\ eV}{\text{joule}}$$

$= 3.06\ eV$

$\Rightarrow \mathcal{E}_w = 1.09\ eV$

1.5. $\frac{d\mathcal{E}}{dt} = \frac{-2e^2(\ddot{r})^2}{3c^3}$

$r = a \sin \omega t$

$\Rightarrow \ddot{r} = -a\omega^2 \sin \omega t$

$\Rightarrow \frac{d\mathcal{E}}{dt} = \frac{-2e^2a^2\omega^4}{3c^3} \sin^2 \omega t$

$\mathcal{E} = \frac{-2e^2a^2\omega^4}{3c^3}\left[\frac{1}{2}t - \frac{1}{4\omega}\sin 2\omega t\right]$

$\bar{\mathcal{E}} = \frac{-2e^2a^2\omega^4 t}{6c^3}$

$\frac{d\bar{\mathcal{E}}}{dt} = \frac{-2e^2a^2\omega^4}{6c^3}$

FOR HARMONIC OSCILLATOR:

$\omega^2 = \frac{\gamma}{m_o}, \quad a^2 = \frac{2E}{\gamma}$

$\Rightarrow \omega^2 a^2 = \frac{2E}{m_o}$

$\Rightarrow \frac{d\mathcal{E}}{dt} = \frac{-2e^2\omega^2}{3m_oc^3}E$

A DIFFERENTIAL EQUATION OF THE FORM $\frac{dV}{dt} = -\frac{1}{\tau}V$

HAS SOLUTION $V = e^{-\frac{1}{\tau}t}$ $\ni$ τ = DECAY CONSTANT.

APPLYING THIS ANALOGY TO THE ABOVE RELATIONSHIP:

$\tau = \frac{3m_oc^3}{2e^2\omega^2}$

$= \frac{3(9.11\times10^{-28}\,\text{GRAM})(3.00\times10^{10}\,\frac{\text{cm}}{\text{SEC}})^3}{2(4.80\times10^{-10}\,\text{esu})^2\omega^2}$ (IN CGS)

$= \frac{1.60\times10^{23}}{\omega^2}$

$\omega = 10^{15}\,\frac{\text{RAD}}{\text{SEC}} \times \frac{1\,\text{CYC}}{2\pi\,\text{RAD}} = \frac{10^{15}}{2\pi}\,\frac{\text{CYC}}{\text{SEC}}$

$\Rightarrow \tau = 6.32\times10^{-7}\,\text{SEC}$

$\omega = \frac{10^{10}}{2\pi}\,\frac{\text{CYC}}{\text{SEC}}$

$\Rightarrow \tau = 6.32\times10^{3}\,\text{SEC}$

1.7. $V = \dfrac{1.24\times10^{4}}{\lambda\,(\text{in }\mathring{A})}$ EQ. 1.8

$$\frac{1}{\lambda} = R_H\left(\frac{1}{K^2} - \frac{1}{n^2}\right)$$

FOR IONIZATION, $\frac{1}{\lambda} = R_H = 109677/\text{cm}$

$$\Rightarrow V = \frac{1.24\times10^{4}\times109677}{\text{cm}\times10^{8}\mathring{A}/\text{cm}} =$$

$$= 13.6\text{eV} \qquad \left(\times\frac{1\text{ joule}}{6.24\times10^{18}\text{eV}}\times\frac{1.6\times10^{-19}\text{ coul}}{\text{electron}}\times\frac{1\text{V}}{\text{coul}} = 3.5\times10^{-37}\right)$$

$V = 1.89\text{eV}$.

$$\frac{1}{\lambda} = R_H\left(\frac{1}{K^2} - \frac{1}{n^2}\right)$$

$$V = \frac{1.24\times10^{4}}{\lambda\,(\mathring{A})}$$

$$\Rightarrow \frac{1}{\lambda(\text{in }\mathring{A})} = \frac{V}{1.24\times10^{4}} = R_H\left(\frac{1}{K^2} - \frac{1}{n^2}\right)$$

$$R_H = 109677\,\frac{1}{\text{cm}}\times\frac{1\text{ cm}}{10^{8}\mathring{A}} = 1.09677\times10^{-3}\mathring{A}$$

$$\Rightarrow \frac{1}{K^2} - \frac{1}{n^2} = \frac{1.89}{(1.24\times10^{4})(1.09677\times10^{-3})} = 1.389$$

THIS RELATIONSHIP IS SATISFIED FOR

$K = 2$ AND $n = 3$

$\Rightarrow$ THE CURRENT DROP REPRESENTS AN ELECTRON CHANGING FROM ITS SECOND TO ITS THIRD LOWEST ENERGY LEVEL.

1.11. $\lambda - \lambda_0 = \dfrac{h(1-\cos\theta)}{m_0 c}$ Eq. 1.12

$$p^2 = \hbar^2(K_0^2 + K^2 - 2K_0 K \cos\theta) \qquad \text{Eq. 1.11}$$

$$K = \frac{2\pi}{\lambda}, \quad \nu = \frac{c}{\lambda}$$

$$h\nu_0 + m_0c^2 = h\nu + (m_0^2c^4 + p^2c^2)^{\frac{1}{2}} \qquad \text{Eq. 1.9}$$

SOLVING FOR p^2 IN Eq. 1.9

$$p^2 = \frac{1}{c^2}\left[(h\nu_0 + m_0c^2 - h\nu)^2 - m_0^2c^4\right]$$

EQUATING WITH Eq. 1.11:

$$c^2\hbar^2\left[K_0^2 + K^2 - 2K_0K\cos\theta\right] = (h\nu_0 + m_0c^2 - h\nu)^2 - m_0^2c^4$$

$$= c^2h^2\left(\frac{1}{\lambda_0^2} + \frac{1}{\lambda^2} - \frac{2\cos\theta}{\lambda\lambda_0}\right) = c^2h^2\,\frac{\lambda^2 + \lambda_0^2 - 2\lambda\lambda_0\cos\theta}{\lambda_0^2\lambda^2}$$

NOW, SINCE $\nu = \frac{c}{\lambda}$

$$\left(\frac{hc}{\lambda_0} + mc^2 - \frac{hc}{\lambda}\right)^2 - m_0^2c^4 = \left[hc\left(\frac{1}{\lambda_0} - \frac{1}{\lambda}\right) + m_0c^2\right]^2 - m_0^2c^4$$

$$= h^2c^2\left(\frac{\lambda^2 + \lambda_0^2 - 2\lambda\lambda_0}{\lambda^2\lambda_0^2}\right) + \frac{2mc^3h(\lambda-\lambda_0)}{\lambda\lambda_0}$$

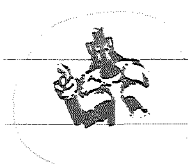
$$= c^2h^2\,\frac{\lambda^2 + \lambda_0^2 - 2\lambda\lambda_0\cos\theta}{\lambda_0^2\lambda^2}$$

OR $h^2c^2\dfrac{-2}{\lambda\lambda_0} + \dfrac{2mc^3h(\lambda-\lambda_0)}{\lambda\lambda_0} = \dfrac{-2c^2h^2\cos\theta}{\lambda\lambda_0}$

$$h^2c^2 - mc^3h(\lambda - \lambda_0) = +c^2h^2\cos\theta$$

$$mc^3h(\lambda - \lambda_0) = c^2h^2(1 - \cos\theta)$$

$$\Rightarrow \lambda - \lambda_0 = \frac{h(1-\cos\theta)}{m_0c}$$



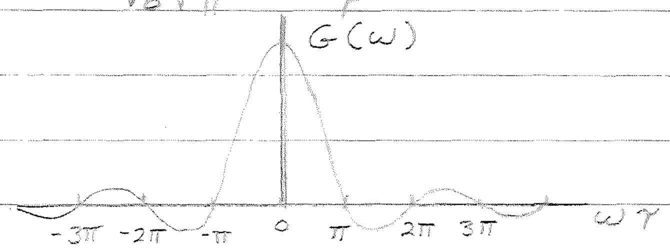
1.15. $V(t) = V_0 \,\mathrm{rect}\left[\frac{t}{2\tau}\right]$

$$\Rightarrow G(\omega) = \sqrt{\frac{2}{\pi}} \int_0^\infty V(t)\cos\omega t \, dt$$

$$= \sqrt{\frac{2}{\pi}} \int_0^\tau V_0 \cos \omega t \, dt$$

$$= \sqrt{\frac{2}{\pi}} \frac{V_0}{\omega} \sin \omega t \Big|_0^\tau$$

$$= V_0 \sqrt{\frac{2}{\pi}} \frac{\sin \omega\tau}{\tau}$$



(TRACED FROM FIG 1.7b)

DEFINE $\frac{\Delta\omega}{2}$ SUCH THAT

$$G\left(\frac{\Delta\omega}{2}\right) = \left(\frac{2}{\pi}\right) G(0) \qquad G(0) = \tau V_0 \sqrt{\frac{2}{\pi}}$$

$$\Rightarrow G\left(\frac{\Delta\omega}{2}\right) = V_0 \sqrt{\frac{2}{\pi}} \frac{\sin \frac{\Delta\omega\tau}{2}}{\Delta\omega/2} = \left(\frac{2}{\pi}\right)^{3/2} V_0 \tau$$

$$\therefore \frac{\sin \Delta\omega\tau/2}{\Delta\omega/2} = \frac{2\tau}{\pi}$$

DEFINE $\Delta\nu = \frac{\Delta\omega}{2\pi}$ OR $\Delta\omega = 2\pi\Delta\nu$

$$\Rightarrow \frac{\sin \pi\Delta\nu\tau}{\pi\Delta\nu} = \frac{2\tau}{\pi}$$

$$\text{OR} \quad \frac{\sin \pi\Delta\nu\tau}{\Delta\nu} = 2\tau$$

DEFINE $\Delta t = 2\tau$

$$\Rightarrow \frac{\sin \pi\Delta\nu\Delta t/2}{\Delta\nu} = \Delta t$$

$$\text{OR} \quad \sin \frac{\pi\Delta\nu\Delta t}{2} = \Delta\nu\Delta t$$

THIS RELATIONSHIP IS VALID ONLY FOR $\Delta\nu\Delta t = 0$, (WHICH IS A NO-NO SOLUTION) OR $\Delta\nu\Delta t = 1$

6. ENERGY LEVEL DIAGRAM FOR BOHR ATOM

$$E(ev) = \frac{1.24\times 10^4\ ev\text{-}\AA}{\lambda}$$

$$\frac{1}{\lambda(cm)} = 1.10\times 10^5\left(\frac{1}{K^2}-\frac{1}{n^2}\right)\frac{1}{cm}$$

$$\Rightarrow E(ev) = 1.10\times10^5\times1.24\times10^4\ \frac{\AA\text{-}ev}{cm}\times\frac{1\,cm}{10^8\,\AA}\left(\frac{1}{K^2}-\frac{1}{n^2}\right)$$

$$= 13.6\ ev\left(\frac{1}{K^2}-\frac{1}{n^2}\right)$$

$$E_n = -\frac{13.6}{n^2}\ ev$$

$E_1 = -13.6\ ev$

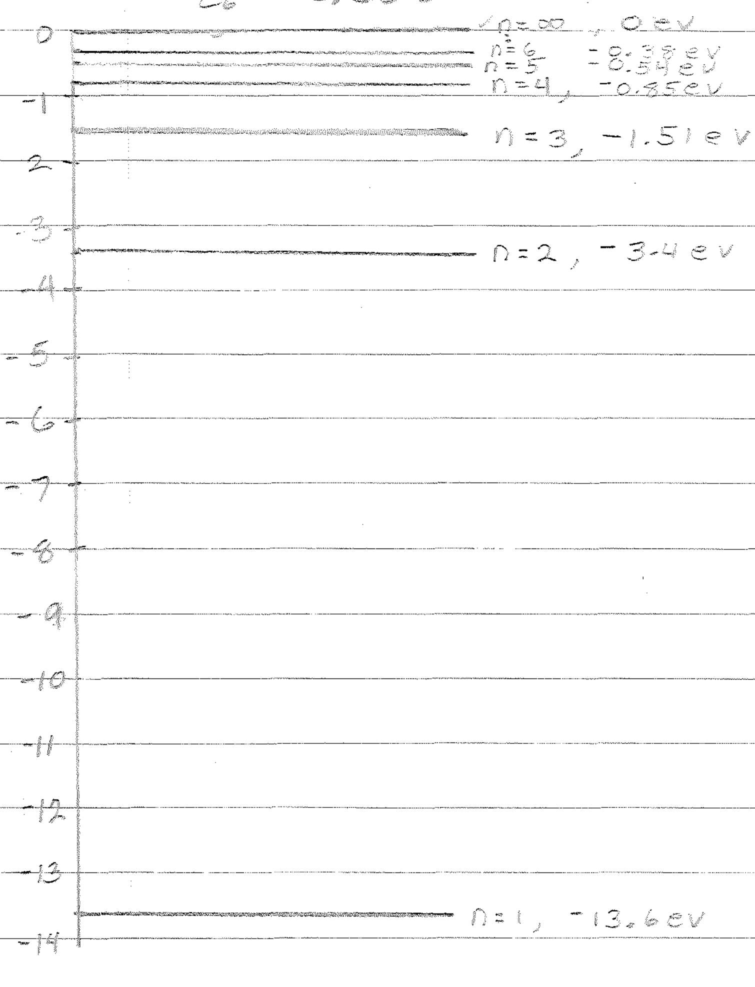
$E_2 = -3.40\ ev$

$E_3 = -1.51\ ev$

$E_4 = -0.85\ ev$

$E_5 = -0.54\ ev$

$E_6 = 0.38\ ev$ ETC



$f_j \triangleq P[\text{ELECTRON IS IN STATE } j]$

ASSUME 1 ELECTRON PER ACCEPTOR

$f_j = P[\text{"HOLE" IS IN STATE } j]$ (PT h HAS ENERGY E_j)

$$f_j = \left[1 + \sum_{i \neq j} f_i\right] \frac{1}{\left[1 + e^{(E_F - E_a - E_j)/kT}\right]}$$

$$\frac{1}{kT}(E_F - E_a - E_j) = \theta_a$$

$$f_j = \left[1 + f_j - \sum f_i\right] \, {}^{1}/_{1+e^{\theta_a}}$$

$$f_j\left[1 - \frac{1}{1+e^{\theta_a}}\right] = \left[1 - \sum f_i\right]\left({}^{1}/_{1+e^{\theta_a}}\right)$$

$$= F^+ \left(\frac{1}{1+e^{\theta_a}}\right)$$

$F^+ = P[\text{ACCEPTOR ATOM HAS NO HOLE}]$

$$f_j = F_+ e^{\theta_a}$$

$F_0 + F_+ = 1 \Rightarrow F_0 = P[\text{ACCEPTOR HAS A HOLE}]$

$$= \sum f_i$$

$$F^+\left(1 + \sum e^{-\theta_a^i}\right) = 1$$

$$\Rightarrow F^+ = \frac{1}{1 + \sum e^{-\theta_a}} = \frac{n_a}{N_A}$$

n_a = # HOLES IN CONDUCTION BAND FROM ACCEPT.

N_A = CONCENTRATION OF ACCEPTOR ATOMS

TO INCLUDE DEGENERACY LET g_j = # STATES W/E = E_j

$$\Rightarrow F^+ = \left[1 + \sum_j g_j e^{-\theta_a}\right]^{-1}$$

$$\simeq \left[1 + g_{grd} e^{-\theta_{a\,grd}}\right]^{-1}$$

$$\Rightarrow F_0 = 1 - F^+ = \frac{1}{1 + \frac{1}{g_{grd}} e^{\theta_{grd}}}$$

AT $j = 1$: $F_0 = \left[1 + \frac{1}{g} e^{(E_F - E_a)/kT}\right]^{-1}$

$$F^+ = \left[1 + g\, e^{(E_F - E_a)/kT}\right]^{-1}$$

ETC.

BOB MARKS

EFFECTIVE MASS IN 3 DIMENSIONS

$$\frac{\delta \vec{V}}{\delta t} = \overleftrightarrow{m}^{-1} \vec{F}$$

$\overleftrightarrow{m}^{-1}$ = RECIPRICAL EFFECTIVE MASS TENSOR

$$\frac{\delta V_i}{\delta t} = m^{-1}_{ij} F_j$$

$$\frac{\delta V_i}{\delta t} = \frac{\delta V_i}{\delta K_j} \frac{\delta K_j}{\delta t} = \frac{F_j}{\hbar} \frac{\delta V_i}{\delta K_j}$$

$$\Rightarrow m^{-1}_{ij} = \frac{1}{\hbar} \frac{\delta V_i}{\delta K_j}$$

NOW $\vec{V} = \nabla_k \omega \quad \Rightarrow \quad \vec{\nabla}_k = \frac{\delta}{\delta K_x}\vec{a}_x + \frac{\delta}{\delta K_y}\vec{a}_y + \frac{\delta}{\delta K_z}\vec{a}_z$

$$\omega = \frac{1}{\hbar} E$$

$$\Rightarrow \vec{V} = \frac{1}{\hbar} \vec{\nabla}_k E$$

$$V_i = \frac{1}{\hbar} \frac{\delta}{\delta K_i} E$$

$$\frac{dV_i}{\delta K_j} = \frac{1}{\hbar} \frac{\delta^2 E}{\delta K_i \delta K_j}$$

$$\Rightarrow m^{-1}_{ij} = \frac{1}{\hbar^2} \frac{\delta^2 E}{\delta K_i \delta K_j}$$

$$m_{ij} = \frac{\hbar^2}{\delta^2 E / \delta K_i \delta K_j}$$

$$\begin{bmatrix} m_{xx} & m_{xy} & m_{xz} \\ m_{yx} & m_{yy} & m_{yz} \\ m_{zx} & m_{zy} & m_{zz} \end{bmatrix} = \hbar^2 \begin{bmatrix} \frac{\delta^2}{\delta K_x^2} & \frac{\delta^2}{\delta K_x \delta K_y} & \frac{\delta^2}{\delta K_x \delta K_z} \\ \frac{\delta^2}{\delta K_y \delta K_x} & \frac{\delta^2}{\delta K_y^2} & \frac{\delta^2}{\delta K_y \delta K_z} \\ \frac{\delta^2}{\delta K_z \delta K_x} & \frac{\delta^2}{\delta K_z \delta K_y} & \frac{\delta^2}{\delta K_z^2} \end{bmatrix} E$$

BOB MARKS
5313
H.W. #3
10-8-75

$$\frac{d\vec{v}}{dt} = \overleftrightarrow{m}^{-1}\vec{F} \Rightarrow \overleftrightarrow{m}^{-1} = \text{RECIPRICAL EFFECTIVE MASS TENSOR}$$

$$\frac{dv_i}{dt} = m_{ij}^{-1} F_j$$

$$\frac{dv_i}{dt} = \frac{\delta v_i}{\delta k_j}\frac{\delta k_j}{\delta t}$$

$$= \frac{F_j}{\hbar}\frac{\delta v_i}{\delta k_j} \Rightarrow m_{ij}^{-1} = \frac{1}{\hbar}\frac{\delta v_i}{\delta k_j}$$

NOW: $\vec{V} = \vec{\nabla}_k \omega \quad \Rightarrow \quad \vec{\nabla}_k = \frac{\delta}{\delta k_x}\vec{a}_x + \frac{\delta}{\delta y}\vec{a}_y + \frac{\delta}{\delta z}\vec{a}_z$

$$E = \hbar\omega$$

$$\Rightarrow \vec{V} = \frac{1}{\hbar}\vec{\nabla}_k E$$

$$V_i = \frac{1}{\hbar}\frac{\delta}{\delta k_i}E$$

$$\frac{\delta V_i}{\delta k_j} = \frac{1}{\hbar}\frac{\delta^2 E}{\delta k_i \delta k_j}$$

$$\Rightarrow m_{ij}^{-1} = \frac{1}{\hbar^2}\frac{\delta^2 E}{\delta k_i \delta k_j}$$

$$m_{ij} = \frac{\hbar^2}{\delta^2 E / \delta k_i \delta k_j}$$

$$\begin{bmatrix} \frac{1}{m_{xx}} & \frac{1}{m_{xy}} & \frac{1}{m_{xz}} \\ \frac{1}{m_{yx}} & \frac{1}{m_{yy}} & \frac{1}{m_{yz}} \\ \frac{1}{m_{zx}} & \frac{1}{m_{zy}} & \frac{1}{m_{zz}} \end{bmatrix} = \frac{1}{\hbar^2}\begin{bmatrix} \frac{\delta^2}{\delta k_x^2} & \frac{\delta^2}{\delta k_x \delta k_y} & \frac{\delta^2}{\delta k_x \delta k_z} \\ \frac{\delta^2}{\delta k_y \delta k_x} & \frac{\delta^2}{\delta k_y^2} & \frac{\delta^2}{\delta k_y \delta k_z} \\ \frac{\delta^2}{\delta k_z \delta k_x} & \frac{\delta^2}{\delta k_z \delta k_y} & \frac{\delta^2}{\delta k_z^2} \end{bmatrix} E$$

BOB MARKS
10-10-75
SOLIDS

TWO DIMENSIONAL DENSITY OF STATES

$n^{(1)} = \sqrt{2m}\,\frac{L}{\hbar\pi}\,\sqrt{E}$

$dn^{(1)} = \sqrt{\frac{m}{2}}\,\frac{L}{\hbar\pi}\,\frac{1}{\sqrt{E}})\,dE$

IN THREE DIMENSIONS

$$dn^{(3)} = \frac{1}{8}\left(4\pi n^2\right)dn$$

$$= \frac{1}{8}\left(4\pi\,\frac{2mL^2}{\hbar^2\pi^2}\,E\right)\left(\sqrt{\frac{m}{2}}\,\frac{L}{\hbar\pi}\,\frac{1}{\sqrt{E}}\right)dE$$

$$= \frac{m^{3/2}}{\sqrt{2}}\,\frac{L^3}{\hbar^3\pi^2}\,\sqrt{E}\,dE$$

$$= \frac{1}{\pi^2}\left(\frac{\sqrt{m}\,L}{\hbar}\right)^3\sqrt{E}\,dE$$

IN TWO DIMENSIONS

$$dn^{(2)} = \frac{1}{4}\left(2\pi n\right)dn$$

$$= \frac{1}{4}\left(2\pi\,\sqrt{2m}\,\frac{L}{\hbar\pi}\,\sqrt{E}\right)\left(\sqrt{\frac{m}{2}}\,\frac{L}{\hbar\pi}\,\frac{1}{\sqrt{E}}\right)dE$$

$$= \frac{m}{2\pi}\left(\frac{L}{\hbar}\right)^2 dE$$

$$\Rightarrow dn^{(2)} = \frac{m}{2\pi}\left(\frac{L}{\hbar}\right)^2 dE$$

BOB MARKS
OCT. 15, 1975

SOLVE

$$n(E) = A\int_{E_c}^{\infty} \sqrt{E-E_c}\, e^{-(E-E_F)/kT}\, dE$$

? WHERE A IS CONSTANT

$$n(E) = A\int_{E_c}^{\infty} \sqrt{E-E_c}\, e^{-E/kT}\, dE\, e^{E_F/kT}$$

$$= A\int_{E_c}^{\infty} \sqrt{E-E_c}\, e^{-(E-E_c)/kT}\, dE\, e^{-(E_c-E_F)/kT}$$

LET $\xi = \sqrt{\frac{E-E_c}{kT}} \Rightarrow d\xi = \frac{dE}{2\sqrt{kT}\sqrt{E-E_c}} = \frac{dE}{2kT}\left(\sqrt{\frac{kT}{E-E_c}}\right)$

$d\xi = \frac{dE}{2kT\xi} \Rightarrow dE = 2kT\xi\, d\xi$; $E = E_c \Rightarrow \xi = 0$

$$n(E) = 2kTA\, e^{-\frac{(E_c-E_F)}{kT}} \int_0^{\infty} \xi^2 e^{-\xi^2}\, d\xi$$

$$= 2kTA\, e^{-(E_c-E_F)/kT}\, \frac{\sqrt{\pi}}{4}$$

$$= \frac{\sqrt{\pi}\, kTA}{2}\, e^{-(E_c-E_F)/kT}$$

$$A = \frac{\pi}{2}\left(\frac{2m}{\hbar^2 \pi^2}\right)^{3/2}$$

AT THE BRILLOIN ZONE BOUNDARY*

$$K = \frac{\pi}{2d} = \frac{2\pi}{\lambda}$$

FOR $d = \frac{1}{2}\text{Å} = 0.5 \times 10^{-8}\,cm$,

$$K = \pi \times 10^{8}\ \frac{RAD}{CM} \qquad \left(\frac{1}{\lambda} = 5 \times 10^{7}/cm\right)$$

① $E = 50\,meV$

$$E = h\nu = \hbar\omega = \hbar c K$$

$$\Rightarrow K = \frac{E}{\hbar c} = \frac{50 \times 10^{-3}\,eV}{1.054 \times 10^{-27}\,erg\text{-}sec \cdot 3 \times 10^{10}\,cm/sec} \times \left(\frac{10^{7}\,erg}{JOULE}\right)\left(\frac{1.6 \times 10^{-19}\,J}{eV}\right)$$

$$= \frac{7590}{3}\ \frac{RAD}{cm} = 2502\ \frac{RAD}{CM}$$

② $E = 3\,eV$

$$K = \frac{E}{\hbar c} = \frac{(3\,eV)}{1.054 \times 10^{-27}\,erg\text{-}sec \cdot 3 \times 10^{10}\,cm} \cdot \frac{sec}{} \cdot \frac{10^{7}\,erg}{J} \cdot \frac{1.6 \times 10^{-19}\,J}{eV}$$

$$= \frac{4.554 \times 10^{5}}{3}\ \frac{RAD}{CM}$$

$$= 1.52 \times 10^{5}\ \frac{RAD}{CM}$$

*WANG, pg 121

$$* \ \omega^2 = U'' \left[\left(\frac{1}{M_1} + \frac{1}{M_2} \right) \pm \sqrt{ \left(\frac{1}{M_1} + \frac{1}{M_2} \right)^2 - \frac{4 \sin^2 ka}{M_1 M_2} } \right]$$

$M_1 = M_2 = M$

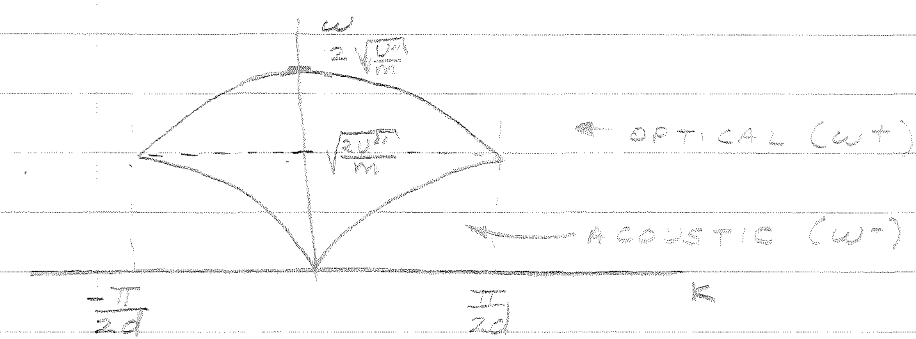
$$\omega^2 = U'' \left[\left(\frac{2}{M} \right) \pm \sqrt{ \left(\frac{2}{M} \right)^2 - \left(\frac{2}{M^2} \right) \sin^2 ka } \right]$$

$$= \frac{2U''}{M} \left[1 \pm \cos ka \right]$$

$$\omega_+^2 = \frac{2U''}{M} (1 + \cos ka) \qquad \omega_-^2 = \frac{2U''}{M} \left[1 - \cos ka \right]$$

$$= \frac{4U''}{M} \cos^2 \frac{ka}{2} \qquad = \frac{4U''}{M} \sin^2 \frac{ka}{2}$$

$$\omega_+ = \pm \sqrt{\frac{4U''}{M}} \cos \frac{ka}{2} \qquad \omega_- = \sqrt{\frac{4U''}{m}} \cdot \sin \frac{ka}{2}$$



V_g = GROUP VELOCITY $= \frac{d\omega}{dK}$

OPTICAL BRANCH:

$$V_g = \pm a \sqrt{\frac{U''}{m}} \sin \frac{ka}{2}$$

ACOUSTIC BRANCH:

$$V_g = \pm a \sqrt{\frac{U''}{M}} \cos \frac{ka}{2}$$

WANG, PG 20, Eq. 2.76

BOB MARKS
SOLIDS
ASSIGNED 10-24-75

$$A_n \phi_n = \psi_n = H_n e^{-\xi^2/2}$$

$$\int_{-\infty}^{\infty} |\phi_n|^2 d\xi = 1$$

$$\int_{-\infty}^{\infty} |\psi_n|^2 d\xi = A_n^2$$

$H_0 = 1$

$$\int_{-\infty}^{\infty} |\psi_0|^2 d\xi = \int_{-\infty}^{\infty} e^{-\xi^2} d\xi = \sqrt{\pi}$$

$H_1 = 2\xi$

$$\int_{-\infty}^{\infty} |\psi_1|^2 d\xi = \int_{-\infty}^{\infty} 4\xi^2 e^{-\xi^2} d\xi = 4 \times \frac{\sqrt{\pi}}{2} = 2\sqrt{\pi}$$

$H_2 = 4\xi^2 - 2$

$$\int_{-\infty}^{\infty} |\psi_2|^2 = \int_{-\infty}^{\infty} (4\xi^2 - 2)^2 e^{-\xi^2} d\xi$$

$$= \int_{-\infty}^{\infty} (16\xi^4 - 8\xi^2 + 4) e^{-\xi^2} d\xi$$

$$= 8\sqrt{\pi} = 2^2 \cdot 2 \cdot \sqrt{\pi}$$

$H_3 = 8\xi^3 - 12\xi$

$$\int_{-\infty}^{\infty} |\psi_3|^2 = \int_{-\infty}^{\infty} (8\xi^3 - 12\xi)^2 e^{-\xi^2} d\xi$$

$$= \int_{-\infty}^{\infty} (64\xi^6 - 192\xi^4 + 144\xi^2) e^{-\xi^2} d\xi$$

$$= 48\sqrt{\pi} = 2^3 (3 \cdot 2) \cdot \sqrt{\pi}$$

$\vdots$

$$H_n = (-1)^n e^{\xi^2} \frac{d^n}{d\xi^n} e^{-\xi^2}$$

$$\int_{-\infty}^{\infty} |\psi_n|^2 = 2^n n! \sqrt{\pi}$$

IT FOLLOWS THAT

$$\int_{-\infty}^{\infty} |\psi_{n+1}|^2 = 2^{n+1} (n+1)! \sqrt{\pi}$$

$$= \int_{-\infty}^{\infty} H_{n+1}^2 e^{-\xi^2} = (2^n n! \sqrt{\pi})\, 2(n+1)$$

$$= 2(n+1) \int_{-\infty}^{\infty} |\psi_n|^2$$

$$= 2(n+1) \int_{-\infty}^{\infty} H_n^2 e^{-\xi^2} d\xi$$

BOB MARKS
SOLIDS
ASSIGNED 10-15-75

WHAT IS C_V AT LARGE TEMP?

$$C_V = \frac{\delta \langle E \rangle}{\delta T} = NK \left(\frac{\hbar\omega}{KT}\right) \times \frac{e^{\hbar\omega/KT}}{\left(e^{\hbar\omega/KT} - 1\right)^2}$$

CONSIDER:

$$e^{\hbar\omega/KT} = 1 + \frac{\hbar\omega}{KT} + \frac{1}{2!}\left(\frac{\hbar\omega}{KT}\right)^2 + \dots$$

FOR LARGE T (AND SINCE $\hbar$ IS SMALL)

$$e^{\hbar\omega/KT} \cong 1 + \frac{\hbar\omega}{KT}$$

AND: $e^{\hbar\omega/KT} - 1 \cong \frac{\hbar\omega}{KT}$

SUBSTITUTING BACK IN

$$C_V \cong NK\left(\frac{\hbar\omega}{KT}\right)\frac{1 + \frac{\hbar\omega}{KT}}{\left(\frac{\hbar\omega}{KT}\right)^2}$$

$$= NK \frac{KT}{\hbar\omega}\left(1 + \frac{\hbar\omega}{KT}\right)$$

$$= NK\left(\frac{KT}{\hbar\omega} + 1\right)$$

BUT UNDER THE ASSUMPTIONS: $\frac{\hbar\omega}{KT} \ll 1$

THUS $\frac{KT}{\hbar\omega} \gg 1$

$\therefore C_V \cong \frac{(NK)KT}{\hbar\omega}$ AT VERY HIGH TEMPERATURES

BOB MARKS
SOLIDS
ASSIGNED 10-27-75

$$P(t) \simeq 4\,|V_{sn}|^2 \rho(E_n) \int_{-\infty}^{\infty} \frac{\sin^2\left[(E_s - E_n)\, t/2\hbar\right]}{(E_s - E_n)^2}\, d(E_s - E_n)$$

$$= 4\,|V_{sn}|^2 \rho(E_n) \int_{-\infty}^{\infty} \frac{\sin^2 \xi t/2\hbar}{\xi^2}\, d\xi$$

$$= 4\,|V_{sn}|^2 \rho(E_n)\, \frac{t^2}{4\hbar^2} \int_{-\infty}^{\infty} \frac{\sin^2 \xi t/2\hbar}{(\xi t/\hbar)^2}\, d\xi$$

$$\eta = \frac{\xi t}{2\hbar} \Rightarrow d\xi = \frac{2\hbar}{t}\, d\eta$$

$$P(t) = 4\,|V_{sn}|^2 \rho(E_n)\, \frac{t}{2\hbar} \int_{-\infty}^{\infty} \frac{\sin^2 \eta}{\eta^2}\, d\eta$$

$$\int_{-\infty}^{\infty} \frac{\sin^2 \eta}{\eta^2} = \pi$$

$$\Rightarrow P(t) = 4\,|V_{sN}|^2 \rho(E_n)\, \frac{t}{2\hbar} \times \pi$$

$$= \frac{2\pi}{\hbar} |V_{sN}|^2 \rho(E_n)\, t$$

BOB MARKS
SOLIDS
ASSIGNED
11-24-75

GIVEN $r_0 = \sqrt{\epsilon}$

$$r^* = r(1 + i\gamma)$$

$$r = \frac{1}{\sqrt{2}}\left[\epsilon + \left(\epsilon^2 + \frac{16\pi^2\sigma^2}{\omega^2}\right)^{\frac{1}{2}}\right]^{1/2}$$

$$\gamma = \sqrt{1 - \epsilon/r^2}\,, \quad \lambda = 5000\,\text{Å}$$

FIND σ SUCH THAT

$$\frac{|r^*| - r_0}{r_0} = \frac{1}{10}$$

$$|r^*| - r_0 = \frac{r_0}{10}$$

$$|r^*| = \frac{11\, r_0}{10}$$

$$|r^*|^2 = \left(\frac{11}{10}\right)^2 r_0^2$$

$$= \left(\frac{11}{10}\right)^2 \epsilon$$

ONWARD:

$$|r^*|^2 = r^2(1 + \gamma^2)$$

$$= r^2\left(1 + \left(1 - \frac{\epsilon}{r^2}\right)\right)$$

$$= r^2\left(2 - \frac{\epsilon}{r^2}\right)$$

$$= 2r^2 - \epsilon$$

THUS: $2r^2 - \epsilon = \left(\frac{11}{10}\right)^2 \epsilon$

$$2r^2 = \left[1 + \left(\frac{11}{10}\right)^2\right]\epsilon$$

$$r^2 = \frac{1}{2}\left[1 + \left(\frac{11}{10}\right)^2\right]\epsilon$$

$$\frac{1}{2}\left[\epsilon + \left(\epsilon^2 + \frac{16\pi^2\sigma^2}{\omega^2}\right)^{1/2}\right] = \frac{1}{2}\left[1 + \left(\frac{11}{10}\right)^2\right]\epsilon$$

$$\epsilon + \left(\epsilon^2 + \frac{16\pi^2\sigma^2}{\omega^2}\right)^{1/2} = \left[1 + \left(\frac{11}{10}\right)^2\right]\epsilon$$

$$\left(\epsilon^2 + \frac{16\pi^2\sigma^2}{\omega^2}\right)^{1/2} = \left(\frac{11}{10}\right)^2\epsilon$$

$$\epsilon^2 + \frac{16\pi^2\sigma^2}{\omega^2} = \left(\frac{11}{10}\right)^4\epsilon^2$$

$$\frac{16\pi^2\sigma^2}{\omega^2} = \left[\left(\frac{11}{10}\right)^4 - 1\right]\epsilon^2$$

$$\sigma^2 = \frac{\omega^2}{16\pi^2}\left[\left(\frac{11}{10}\right)^4 - 1\right]\epsilon^2$$

$$\sigma = \frac{\omega}{4\pi}\sqrt{\left(\frac{11}{10}\right)^4 - 1}\;\epsilon$$

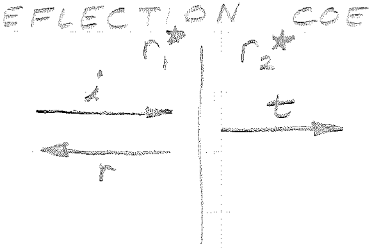
$$\omega = \frac{2\pi c}{\lambda}$$

$$\Rightarrow \sigma = \frac{1}{4\pi}\left(\frac{2\pi c}{\lambda}\right)\sqrt{\left(\frac{11}{10}\right)^4 - 1}\;\epsilon$$

$$= \frac{c\epsilon}{2\lambda}\sqrt{\left(\frac{11}{10}\right)^4 - 1}$$ $\Leftarrow$ NEED TO KNOW ϵ

Bob Marks
Solids
Assigned
11-24-75

REFLECTION COEFFICIENT DERIVATION



INCIDENT

$E_i = E_{io} e^{i\omega t r_1^* \frac{x}{t}}$

$H_i = {}^{+}r_1^* E_{io} e^{i\omega t r_1^* x/t}$

TRANSMITTED

$E_t = E_{to} e^{i\omega t r_2^* x/t}$

$H_t = E_{to} r_2^* e^{+i\omega t r_2^* xt}$

REFLECTED

$E_r = E_{ro} e^{-i\omega t r_1^* xt}$

$H_r = -E_{ro} r_1^* e^{-i\omega t r_1^* xt}$ ⇐ "−" SIGN SINCE POYNTING VECTOR IS TO LEFT

BOUNDARY CONDITIONS:

① $E_i(0) = E_t(0) + E_r(0) \Rightarrow E_{io} = E_{ro} + E_{to}$

② $H_i(0) = H_t(0) + H_r(0) \Rightarrow r_1^* E_{io} = -r_1^* E_{ro} + r_2^* E_{to}$

THEN $E_{to} = \frac{r_1^*}{r_2^*}(E_{io} + E_{ro})$

SUBSTITUTING INTO ①

$$E_{io} = E_{ro} + \frac{r_1^*}{r_2^*}(E_{ro} + E_{io})$$

$$E_{io}\left(1 - \frac{r_1^*}{r_2^*}\right) = E_{ro}\left(1 + \frac{r_1^*}{r_2^*}\right)$$

$$\frac{E_{ro}}{E_{io}} = \frac{1 - r_1^*/r_2^*}{1 + r_1^*/r_2^*} = \frac{r_2^* - r_1^*}{r_2^* + r_1^*}$$

$$R = \left|\frac{E_{ro}}{E_{io}}\right|^2 = \frac{|r_2^* - r_1^*|^2}{|r_2^* + r_1^*|^2} \quad ; \quad r^* = r(1 + i\gamma)$$

$$= \left|\frac{[r_1(1+i\gamma_1) - r_2(1+i\gamma_2)]}{[r_1(1+i\gamma_1) + r_2(1+i\gamma_2)]}\right|^2$$

$$= \frac{|r_1 - r_2 + i(r_1\gamma_1 - r_2\gamma_2)|^2}{|r_1 + r_2 + i(r_1\gamma_1 + r_2\gamma_2)|^2}$$

$$= \frac{(r_1 - r_2)^2 + (r_1\gamma_1 - r_2\gamma_2)^2}{(r_1 + r_2)^2 + (r_1\gamma_1 + r_2\gamma_2)^2}$$

BOB MARKS

① SPECIAL CASE : $\sigma = 0$

$$\Rightarrow r_1 = \sqrt{\epsilon_1}\ ,\ r_2 = \sqrt{\epsilon_2}$$

$$\gamma_1 = 0\ ,\ \gamma_2 = 0$$

$$\therefore R = \left(\frac{\sqrt{\epsilon_1} - \sqrt{\epsilon_2}}{\sqrt{\epsilon_1} + \sqrt{\epsilon_2}}\right)^2$$

② SPECIAL CASE : VACUUM/METAL INTERFACE

MEDIUM 1 : VACUUM : $r_1 = \sqrt{\epsilon_0}$ $\sigma_1 = 0,\ \gamma_1 = 0$

MEDIUM 2 : METAL : ϵ_2, σ_2

$$\gamma_2 = \sqrt{1 - \epsilon/r^2}$$

$$r_2 = \frac{1}{\sqrt{2}}\sqrt{\epsilon_2 + \left(\epsilon_2^2 + \frac{16\pi^2\sigma_2^2}{\omega^2}\right)^{\frac{1}{2}}}$$

AND

$$R = \frac{(\sqrt{\epsilon_1} - r_2)^2 + (r_2\gamma_2)^2}{(\sqrt{\epsilon_1} - r_2)^2}$$

BOB MARKS
SOL105
ASSIGN. 11/25

XAA

IN A HOMOGENEOUS ISOTROPIC MEDIA OF PER. μ, DIELECTRIC CONSTANT ϵ, AND CONDUCTIVITY σ, TWO OF MAXWELL'S EQUATIONS ARE

$$\nabla \times \vec{H} = \epsilon \frac{\delta \vec{E}}{\delta t} + \vec{J}$$

$$\nabla \times \vec{E} = -\delta B / \delta t$$

BUT $\vec{J} = \sigma \vec{E}$ AND $\vec{B} = \mu \vec{H}$

$$\Rightarrow \nabla \times \vec{H} = \epsilon \frac{\delta \vec{E}}{\delta t} + \sigma \vec{E} \quad (1)$$

$$\vec{\nabla} \times \vec{E} = -\mu\, \delta H / \delta t \quad (2)$$

TAKING THE CURL OF (2): (WITH VECTOR IDENTITY)

$$\vec{\nabla} \times \vec{\nabla} \times \vec{E} = \nabla \nabla \cdot \vec{E} - \nabla^2 \vec{E}$$

ASSUMING NO FREE CHARGE IN CONDUCTOR: $\vec{\nabla} \cdot \vec{E} = 0$

$$\Rightarrow \vec{\nabla} \times \vec{\nabla} \times \vec{E} = -\nabla^2 E = -\mu \frac{\delta}{\delta t} \vec{\nabla} \times \vec{H}$$

$$\Rightarrow \frac{\delta}{\delta t} \vec{\nabla} \times \vec{H} = +\frac{1}{\mu} \nabla^2 \vec{E} \quad (3)$$

FROM (1):

$$\frac{\delta}{\delta t} \vec{\nabla} \times \vec{H} = \epsilon \frac{\delta^2 \vec{E}}{\delta t^2} + \sigma \frac{\delta}{\delta t} \vec{E} \quad (4)$$

EQUATING (3) AND (4):

$$\frac{1}{\mu} \nabla^2 \vec{E} - \epsilon \frac{\delta^2 E}{\delta t^2} = \sigma \frac{\delta}{\delta t} \vec{E}$$

$$\nabla^2 E - \epsilon \mu \frac{\delta^2 E}{\delta t^2} = \sigma \epsilon \frac{\delta}{\delta t} E$$

BUT $C^2 = \frac{1}{\mu \epsilon}$

$$\Rightarrow \nabla^2 \vec{E} - \frac{1}{C^2} \frac{\delta^2 E}{\delta t^2} = \frac{\sigma}{C^2 \mu} \frac{\delta}{\delta t} \vec{E}$$

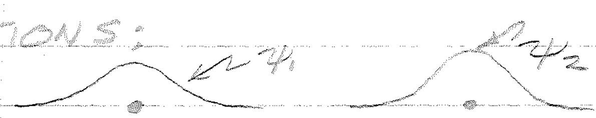
THIS IS THE DESIRED RESULT.

BOB MARKS
SOLIDS
ASSIGN 11/25

<u>TIGHT</u> <u>BINDING APPROXIMATION</u> <u>FOR</u> <u>ELECTRONS IN METALS</u>

THE TIGHT BINDING APPROXIMATION IS GOOD FOR THE INNER ELECTRONS OF BUT IS NOT PARTICULARY GOOD FOR CONDUCTION ELECTRONS. ROUGHLY, THE METHOD STARTS WITH THE WAVE FUNCTIONS OF A NUMBER OF FREE NUETRAL ATOMS. AS THE ATOMS MOVE TOWARDS EACH OTHER (IN A MENTAL PICTURE), THE WAVE FUNCTIONS OVERLAP. ONE THEN LOOKS AT ALL LINEAR COMBINATIONS OF THE BINDED ATOM'S WAVE FUNCTIONS AND COMPUTES THE RESULTING ALLOWABLE ENERGY LEVELS.

AS AN EXAMPLE, CONSIDER THE FOLLOWING SKETCH OF TWO IDENTICAL ATOMS WITH CORRESPONDING WAVE FUNCTIONS:



SUCH A REPRESENTATION IS CHARACTERISTIC OF, SAY, TWO HYDROGEN ATOMS AT THE GROUND STATE. AS THE ATOMS MOVE CLOSER TOGETHER, THE WAVE FUNCTIONS OVERLAP TO GIVE TWO POSSIBLE WAVE FUNCTION COMBINATIONS:

AL

$$\phi_+ \propto \psi_1 + \psi_2$$

$$\phi_- \propto \psi_1 - \psi_2$$

"$\propto$" IS READ "PROPORTIONAL TO"
(PROPORTIONALITY CONSTANT DETERMINED VIA NORMALIZATION)

MEN... COMPU...

BOB MARKS
50L105
ASSIGN 11/25

EXTRA

DISCUSSION OF EXCHANGE TERM

FOR EASE OF DISCUSSION, CONSIDER FIRST, HARTREE'S TWO ELECTRON WAVE FUNCTION: $\psi_1(x_1, x_2) = \phi_1(x_1)\phi_2(x_2)$. THIS RELATIONSHIP ASSUMES TWO STATES (ϕ_1, ϕ_2) AND TWO ELECTRONS RESPECTIVELY AT "POSITIONS" x_1 AND x_2. IT ASSUMES THE ELECTRONS ARE DISTINGUISHABLE. THAT IS, ELECTRON ONE IS ALWAYS IN STATE ϕ_1 AND ELECTRON TWO IS ALWAYS IN STATE ϕ_2. THE CHOICE OF THIS PRODUCT FORM DOES NOT ALLOW ONE TO TAKE INTO ACCOUNT THE CORRELATION IN THE IN THE MOTION OF THE ELECTRONS. FOCH'S METHOD ALLOWS SUCH A TREATMENT. WE HAVE:

$$\psi_2(x_1, x_2) = \frac{1}{2}\left[\phi_1(x_1)\phi_2(x_2) - \phi_1(x_2)\phi_2(x_1)\right].$$

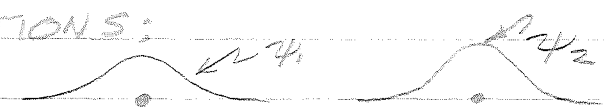
HERE, WE TAKE INTO ACCOUNT ALL POSSIBLE OCCURANCES, ELECTRON ONE IN STATE ONE AND ELECTRON TWO IN STATE TWO OR ELECTRON TWO IN STATE ONE AND ELECTRON ONE IN STATE TWO, BUT NOT BOTH AT ONCE (THIS, OF COURSE, IS DUE TO PAULI'S EXCLUSION PRINCIPLE). IN A VERY ROUGH SENSE, FOCH'S EXPRESSION IS THE PROBABILISTIC SUM ON MUTUALLY EXCLUSIVE EVENTS DISCARDING TERMS SUCH AS $\phi_1(x_1)\phi_1(x_2)$ WHICH VIOLATE THE EXCLUSION PRINCIPLE AND TERMS SUCH AS $\phi_1(x_1)\phi_2(x_1)$ WHICH VIOLATE REASON.

BOB MARKS
SOLIDS
ASSIGN 11/25

<u>TIGHT BINDING APPROXIMATION FOR ELECTRONS IN METALS</u>

THE TIGHT BINDING APPROXIMATION IS GOOD FOR THE INNER ELECTRONS OF ATOMS, BUT IS NOT PARTICULARY GOOD FOR CONDUCTION ELECTRONS. ROUGHLY, THE METHOD STARTS WITH THE WAVE FUNCTIONS OF A NUMBER OF FREE NUETRAL ATOMS. AS THE ATOMS MOVE TOWARDS EACH OTHER (IN A MENTAL PICTURE), THE WAVE FUNCTIONS OVERLAP. ONE THEN LOOKS AT ALL LINEAR COMBINATIONS OF THE BINDED ATOM'S WAVE FUNCTIONS, AND COMPUTES THE RESULTING ALLOWABLE ENERGY LEVELS.

AS AN EXAMPLE, CONSIDER THE FOLLOWING SKETCH OF TWO IDENTICAL ATOMS WITH CORRESPONDING WAVE FUNCTIONS:

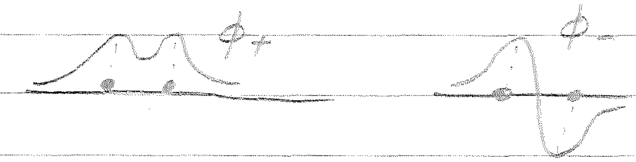


SUCH A REPRESENTATION IS CHARACTERISTIC OF, SAY, TWO HYDROGEN ATOMS AT THE GROUND STATE. AS THE ATOMS MOVE CLOSER TOGETHER, THE WAVE FUNCTIONS OVERLAP TO GIVE TWO POSSIBLE WAVE FUNCTION COMBINATIONS:

$$\phi_+ \propto \psi_1 + \psi_2$$
$$\phi_- \propto \psi_1 - \psi_2$$

"$\propto$" IS READ "PROPORTIONAL TO"
(PROPORTIONALITY CONSTANT DETERMINED VIA NORMALIZATION)

SKETCHES OF THESE FUNCTIONS ARE ROUGHLY



CONSIDER FIRST, ϕ_+. THE ELECTRON WILL SPEND MUCH OF ITS TIME MIDWAY BETWEEN THE ATOMS AT A LOWER ENERGY AS COMPARED TO ϕ_- WHERE THE ELECTRON IS NEVER AT THE MIDPOINT. THUS ϕ_+ HAS A LOWER CORRESPONDING ENERGY THAN ϕ_-.

EXTENSION OF THIS METHOD, THEN, TO A LARGE NUMBER OF ATOMS, IS THE TIGHT BONDING APPROXIMATION. AS N ATOMS ARE BOUGHT CLOSE TOGETHER, THERE WILL RESULT N ENERGIES EACH ASSOCIATED WITH ONE OR MORE ENERGY BANDS. ONE MUST GENERALLY ALLOW FOR VARIOUS ORBITALS, ENERGY SPITTING, AND OTHER STUFF IN SUCH A COMPUTATION.

AS MENTIONED, THE TIGHT BAND APPROXIMATION IS "THOUGHT" TO BE QUITE GOOD FOR INNER ELECTRONS OF ATOMS, SUGGESTING THAT COMPUTATION AND THEORY

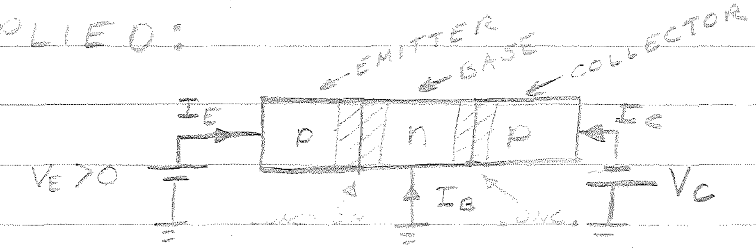
FOR THIS CASE HISTORICALLY AGREE. A SIMILAR STATEMENT HOLDS FOR ITS LESS SUCCESSFUL ROLE IN DESCRIBING CONDUCTION ELECTRONS. IT HAS BEEN EMPLOYED TO APPROXIMATELY DESCRIBE THE d BANDS OF TRANSITION METALS, AND THE VALENCE BANDS OF INERT GAS CRYSTALS.

REF: KITTEL: *INTRODUCTION TO SOLID STATE PHYSICS*

BOB MARKS
SOLIDS
ASSIGNED
12-5-75

EBERS-MOLL MODEL OF TRANSISTOR CURRENT

WE WILL HERE CONSIDER A PNP (JUNCTION) TRANSISTOR FORMED BY JOINING TWO DIODES AT THEIR n JUNCTIONS. BIAS IS APPROPRIATELY APPLIED:



CONSIDER, FIRST, THE FORWARD BIASED EMITTER WHICH INCREASES THE NUMBER OF HOLES IN THE n-DOPED MATERIAL AT THE EMITTER-BASE JUNCTION. THE TOTALITY OF THESE HOLES MAY BE DETERMINED BY A BOLTZMAN FACTOR:

$$P_{TOT} = P_n\left(1 + e^{\frac{e^- V_E}{kT}}\right) \tag{1}$$

WHERE P_n IN THE JUNCTION'S INTRINSIC HOLE DENSITY. WE MAY WRITE EQUIVALENTLY

$$\Delta P_E = P_n\left(e^{e^- V_E/kT} - 1\right) \tag{2}$$

WHERE ΔP_E IS THE "EXCESS" HOLE

DENSITY RESULTING FROM THE FORWARD BIAS VOLTAGE V_E.

IN A SIMILAR FASHION, THE EXCESS HOLE DENSITY AT THE COLLECTOR JUNCTION IS

$$\Delta P_c = P_n \left(e^{e^- V_c/KT} - 1\right) \qquad (3)$$

NOTE, HOWEVER, THAT $V_c < 0$, AND, ACCORDINGLY, $\Delta P_c < 0$.

NOW, A PORTION OF THE HOLES AT THE EMITTER JUNCTION WILL STRAY FROM THE JUCTION AND UNDERGO SOME RECOMBINATION DURING THEIR DIFFUSION. THE ELECTRONS REQUIRED FOR THIS RECOMBINATION ARE SUPPLIED EXTERNALLY BY THE BASE. THUS, CONTROLLING THE BASE CURRENT CONTROLL'S THE AVAILABLE RECOMBINATION ELECTRONS, AND THE NUMBER OF HOLES REACHING THE COLLECTOR IS CONTROLLED BY THE BASE CURRENT.

ASSUMING THE VOLTAGE DROP OCCURS PRIMARILY ACROSS THE JUNCTION, ONE MAY USE BOLTZMAN FACTOR REASONING TO WRITE

$$I_C = -\alpha I_{EO}\left(e^{eV_E/kT} - 1\right) - I_{CO}\left(e^{eV_C/kT} - 1\right)$$

HERE, THE PROPORTIONALITY CONSTANT IS

α = FORWARD CURRENT TRANSPORT FACTOR (CURRENT GAIN)

$$= \frac{\text{EXCESS COLLECTOR CURRENT}}{\text{EMITTER CURRENT}}$$

FOR LARGE VALUES OF BIAS

$$-I_C \simeq \alpha I_E + I_{CO}$$

SIMILARLY THE BASE CURRENT:

$$-I_B = (1-\alpha) I_E - I_{CO}$$

THE TRANSISTOR β IS FOUND FROM

$$-I_C = -\beta I_B + \frac{I_{CO}}{1-\alpha} \; ; \; \beta = \frac{\alpha}{1-\alpha}$$

WE HAVE NOTED THAT A LARGE COLLECTOR CURRENT IS CONTROLLED BY A SMALL BASE CURRENT. THIS BECOMES SMALLER AS α NEARS 1.

IT CAN BE SHOWN THAT, FOR A NARROW BASE REGION ($W_B \ll L_P$):

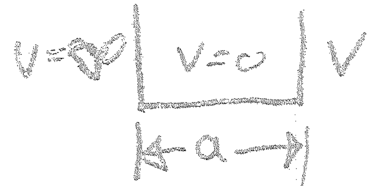
$$\alpha \simeq 1 - (W_B/L_P)^2$$

(1) Set up an expression for the number of holes in the valence band of a semiconductor, assuming pure material. Describe each term.

(2) What is the Fermi energy? How is it determined? What is the effect of doping?

(3) Describe qualitatively the phonon and electron energy level structure of a solid.

(4) Solve the Schroedinger equation for



and obtain an energy formula.

1. h = # HOLES IN THE VALENCE BAND

$= N_V e^{-(E_F - E_V)/KT}$ FOR SMALL T

FROM $h = C \int_{-\infty}^{E_c} h(E)\, dE$

$$h = C \int_{\text{VALENCE BAND}} \frac{\sqrt{E_V - E}}{1 + e^{(E-E_F)/KT}}\, dE$$

C = CONST

$$h \sim C \int_{\text{VALENC BAND}} \sqrt{E_V - E}\; e^{-(E-E_F)/KT}$$ FOR SMALL T

$h(E)$ = DENS. OF STATES

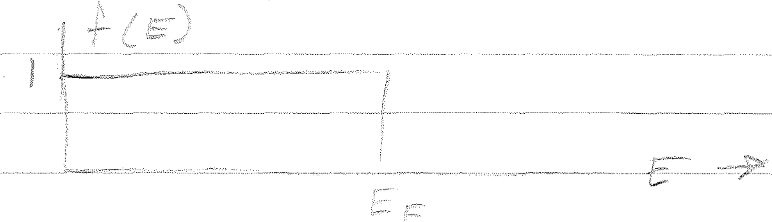
$f(E)$ = FERMI DIRAC DISTRIBUTION

$h(E) = [1 - f(E)]\, p(E)$

$p(E)$ = # HOLES AS A FUNCTION OF E.

2. The Fermi Energy ~~is~~ may be defined as that energy of a solid which at $0°K$, all energy is ~~hifer~~ below it.

~~So~~ At $0°K$ the Fermi Dirac dist. ~~equation~~ looks like:



Doping ~~ch~~ changes the Fermi energy level. Donor doping will increase it and acceptor doping will decrease it.

3. Electrons may only ~~hav~~ have quantized energy. ~~[illegible]~~ Roughly, an electron can be

1. in the valence band (where most e's are)
2. Within an acceptor
3. In the conduction band.

Conduction band

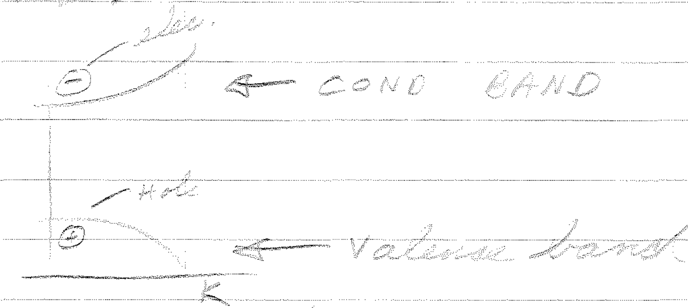
Acc. Level

Valence

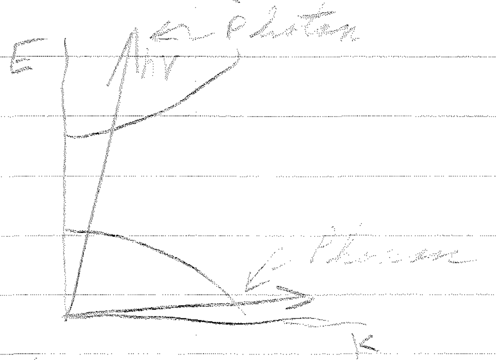
Similarly a hole can be at these places, except at the donor level (instead of accept.)

An electron in the conduction band may combine with a hole in the valence band producing a phonon and a photon.

Before



After

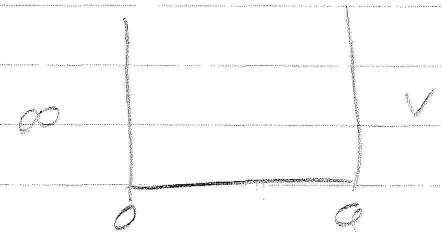


That is:

$$h_{VB} + e_{CB} = P_{h\nu} + \text{PHONON}$$

In this interaction momentum must be conserved. The phonon velocity is very low and the light is is very high.

4.



$$+\frac{\hbar^2}{2M}\frac{\delta^2\psi}{\delta x^2} - E\psi = 0$$

? ? $$\frac{\delta^2\psi}{\delta x^2} - \frac{2mE}{\hbar^2}\psi = 0$$

$$\frac{\delta^2\psi}{\delta x^2} + k^2\psi = 0 \qquad k^2 = \frac{2mE}{\hbar^2}$$

$$\psi = A\cos kx + B\sin kx$$

$$\psi(0) = 0 \Rightarrow A = 0$$

$$\psi = B\sin kx$$

$$\psi(a) = 0 \Rightarrow k = \frac{\pi n}{a}$$

$$\Rightarrow \psi = B\sin kx$$

GET B FROM $\int_0^a B^2 \sin^2 \frac{\pi n x}{a}\, dx = 1$

ANYWAY

$$k^2 = \frac{\pi^2 n^2}{a^2} = \frac{2mE}{\hbar^2}$$

$$\Rightarrow E_n = \frac{\pi^2 n^2 \hbar^2}{2m}$$

5313 1/4/75

Solve $\underline{\underline{4}}$ only

① Give as complete a derivation as possible, making necessary assumptions, of the Wiedemann-Franz ratio for metals

$$\frac{K}{\sigma T} = \frac{\pi^2}{3}\frac{k^2}{e^2}$$

② Consider a lattice of atoms with nearest neighbors at $a(1,1,1)$, $a(1,-1,-1)$, $a(-1,-1,1)$, $a(-1,1,-1)$. Assuming an interaction between nearest neighbors only (for electrons tightly bound), obtain an expression for $\mathcal{E}(k)$. Let $V_{ij} = 1$ for nearest neighbors obtain an expression for the effective mass.

~~③ For a solid with atomic polarizability α, and $n\ \frac{\text{atoms}}{\text{unit vol}}$, the Clausius-Mossotti equation states $\frac{\epsilon-1}{\epsilon+2} = \frac{4\pi n\alpha}{3}$. Derive this.~~

④ Describe heat conduction in an insulator

(5) Derive a dispersion relation for a one-dimension lattice of atoms, mass m, connected by springs, spring constant k, and separated by d.

(6) What would the effect of a light impurity be on the vibrational ~~spectra~~ structure of a solid? assume a impurity, mass m, is in place of an atom of a monoatomic solid, mass M, with $m < M$.

(7) What atoms would you expect to be donors and acceptors in Si?

15 20

1. ONE starts with the Boltzman Transport Equation (a 6-dimensional time variant probability density function PDF) something like

$$\vec{v} \cdot \nabla_r f + \vec{a} \cdot \vec{\nabla}_v f = -(f - f_0)/\tau$$

where f is the PDF and f_0 is the equilibrium PDF. The Weidemann Franz Ratio employs the Fermi-Dirac distribution for f_0

$$f_0 = \left[1 + e^{(E - E_F)/kT}\right]^{-1}$$

where $E = \hbar^2 k^2/2m$ and E_F is the Fermi-energy. You then find J_x, the current density from $J_x = e \iiint_{-\infty}^{\infty} \tau(\quad) v_x \, dv_x dv_y dv_z$ where $(\quad)$ is the equilibrium 1-D PDF (Note: $\int_{-\infty}^{\infty} f_0 \, dv_x dv_y dv_z = 0$)

This gives you something like (From $\frac{dT}{dx} = 0$) $\frac{e^2 n}{m^*}\tau(E_F) = \sigma \doteq \frac{J_x}{E_x} = \sigma$

The thermal current density C_x is analogously computed

$$C_x = - \iiint \tau(\quad) v_x E \, dv_x dv_y dv_z$$

Free electrons are assumed. τ is the relaxation time. The resulting thermal conductivity K is then $K = \frac{\pi^2}{3} \frac{k^2}{m^*} n \, \tau(E_F)$

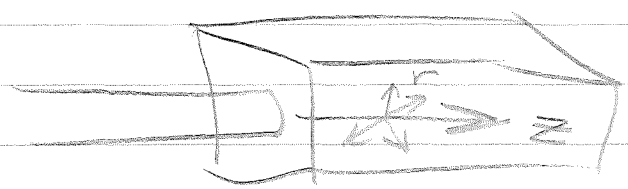
Taking the ratio gives the W-F ratio

$$\frac{K}{\sigma T} = \frac{\pi^2}{3} \frac{k^2}{e^2}$$

4. The diffusion of heat is described by the differential equation:

$$\nabla^2 T = \frac{\rho c}{K}\frac{\delta T}{\delta t}$$

where ρ is the density, c is the specific heat, and K is the thermal conductivity. An example (derived in class) describing heat diffusion ~~was~~ illumination of a material with a Gaussian beam ($I = I_0 e^{-r^2/2r_0^2}$) for a short time and watching how the temper. changes (1) radially and (2) in the z direction.



(1) For the radial case after going through Hankel xforms etc, the final answer was something like

$$T(r,t) = T_0 \alpha e^{-\alpha r^2/\rho r^2}$$

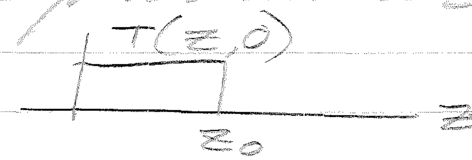
where $\alpha = \left(1 + 2Kt/\rho c r_0^2\right)^{-1}$

that is, the temperature spread outward (in r) at an inverse exponential manner determined by the material's intrinsic constants. We noted that @ $r=0$ $2KT = r_0^2 \rho c$.

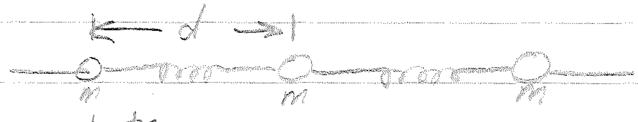
② For the z direction after going through some Fourier cosine x form stuff, we found that (something like)

$$② \quad T(0,t) = T_0 \, \mathrm{erf} \; z_0 \sqrt{\frac{\rho c}{4K}}$$

where z_0 was an initial condition parameter:

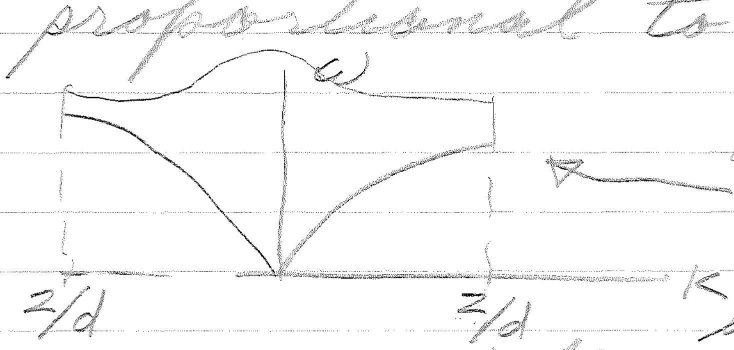


Here again behavior is governed solely by the intrinsic behavior of the material

5. 

$F = kU$ K = SPRING CONSTANT

one considers, to an approximation, interaction of atom n with atoms $n-1$ and $n+1$ (ie Truncated Taylor Series) (ie only with the nearest neighbors.) This gives one two simultaneous differential equations with two arbitrary constants. Taking the determinate and setting to zero wipes out these constants and leaves one with something proportional to sin Kd.



So the first Brillouin zone is. There also exists a light band. The mass m determines the curve's intersection at the Brillouin boundaries.

10

7. A donor in Si would be an element with five electrons in its conduction? shell. Similarly an acceptor should have three electrons in the conduction shell

Bob Marks

1

9-3-75 (WED)

WANG - SOLID STATE ELECTRONICS (TEXT)

REFS: SHOCKLEY - ELECTRONS AND HOLES IN SEMICONDUCTORS

KITTEL - SOLID STATE PHYSICS

R. BUBE - ELECTRONIC PROPERTIES OF CRYSTALLINE SOLIDS

J. C. PHILLIPS - BONDS AND BANDS IN SEMICONDUCTORS

SOLIDS AREAS:

- DEVICES: JUNCTION, FET'S, IC'S, LED'S, JFET'S, IMPATT, SWITCHES, ETC.
- PROPERTIES OF SOLIDS: MAGNETIC, LUMINESCENCE, ELECTRONIC, OPTICAL
- QUANTUM ELECTRONICS: SOLID STATE LASERS, Q-SWITCH, OPTICAL THIN FILMS, INTEGRATED OPTICS
- FUNDAMENTAL PROPERTIES: LATTICE RESONANCE, BAND STRUCTURE, LINEAR AND NONLINEAR INTERACTIONS OF LIGHT WITH MATTER
- DEFECTS AND IMPURITIES: DONORS & ACCEPTORS, DISLOCATIONS, PHONON EXITONS.
- SUPERCONDUCTIVITY: BCS THEORY OF, JOSEPHSON JUNCTION
- SURFACE PROPERTIES:
- THERMAL PROPERTIES:
- METHODS OF STUDY

ELECTRONIC: RESISTIVITY, HALL EFFECT, TRANSPORT

LASERS

MAGNETICS

H.W.: READ TO Pg. 12. IN TEXT

WAVE & PARTICAL NATURE OF MATTER

LIGHT: $E = h\nu$

h = PLANCK'S CONSTANTS

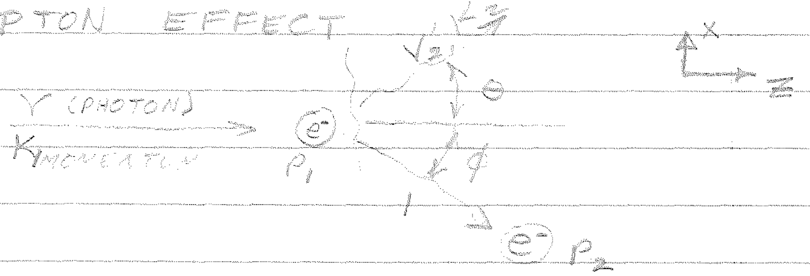
$\vec{p} = h/\lambda$

SCHROEDINGER'S EQ'N

$$\frac{\hbar^2}{2m}\nabla^2\psi + V(\vec{r})\psi = E\psi$$

9-5-75 (THURS)

COMPTON EFFECT



$E_{PHOTON} = h\nu = \hbar\omega$ $\quad P_{PHOTON} = \hbar k \quad \hbar = \frac{h}{2\pi}, \; k = \frac{2\pi}{\lambda}$

λ = WAVELENGTH, K = BOLTZMAN'S CONST, h = PLANCK'S CONST

$\omega = 2\pi\nu$

TO SOLVE, USE RELATIVISTIC KINEMATICS.

4-MOMENTUM

FOR ELECTRON, $[E, P_x, P_y, P_z]$

$[E, P_x, P_y, P_z]\cdot[E, P_x, P_y, P_z] = E^2 - \vec{p}\cdot\vec{p}$

$= E^2 - p^2$

HERE, $\hbar, c \equiv 1 \quad E = m$

$\Rightarrow E^2 - p^2 = m^2 - p^2$

BACK TO PROBLEM:

$k_1 = [\omega_1, 0, 0, \omega_1] \qquad k_2 = [\omega_2, \omega_2 \sin\theta, 0, \omega_2 \cos\theta]$

$P_1 = [m, 0, 0, 0] \qquad P_2 = [E_2, P_2 \sin\phi, 0, P_2 \cos\phi]$

NOW, TO CONSERVE ENERGY:

$P_1 + k_1 = P_2 + k_2 \Rightarrow P_2 = P_1 + K_1 - K_2$

$P_2^2 = [P_1 + K_1 - K_2]^2$

$= P_1^2 + k_1^2 + k_2^2 + 2P_1\cdot k_1 - 2P_1\cdot k_2$

$- 2k_1\cdot k_2$

$$m^2 = m^2 + 0 + 0 + 2P_1\cdot K_1 - 2P_1\cdot K_2 - 2K_1\cdot K_2$$

$$\Rightarrow P_1\cdot K_1 = P_1\cdot K_2 + K_1\cdot K_2$$

$$m\omega_1 = m\omega_2 + \omega_1\omega_2\left[1-\cos\theta\right]$$

$$\therefore \frac{1}{\omega_2} - \frac{1}{\omega_1} = \frac{1}{m}\left[1-\cos\theta\right]$$ $\Leftrightarrow$ COMPTON SCATTERING

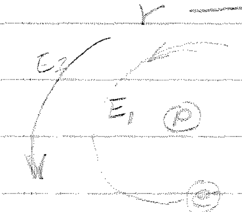
THE BOHR ATOM

HYDROGEN SPECTRA


← CHARACTERISTIC FREQUENCIES

$\nu \longrightarrow$

ATOM



METHOD OF ATTACK

$E_{electron}$

FORCE EQUATION

ANGULAR MOMENTUM

$$E = \underbrace{\frac{1}{2}mv^2}_{K.E.} + \underbrace{\frac{Ze^2}{4\pi\epsilon r}}_{POTENTIAL}$$

COULOMB FORCE MUST EQUAL MECHANICAL FORCE

$$\frac{mv^2}{r} = \frac{Ze^2}{4\pi\epsilon r^2}$$

L = ANGULAR MOMENTUM

$= m\vec{r}\times\vec{v} = mrv \quad (= n\hbar)$

FROM PLANCK'S WORK BOHR KNEW LIGHT OF FREQ. ν HAD ENERGY $E = h\nu$

AND, FROM DISCRETE ORBITS ASSUMPTION: $E_2 - E_1 = h\nu$

$\Rightarrow L = n\hbar$

SO IMPORTANT EQUATIONS:

$E = \frac{1}{2}mv^2 + \frac{Ze^2}{4\pi\epsilon r}$ ⇐ CONSER. OF E

$\frac{mv^2}{r} = \frac{-Ze^2}{4\pi\epsilon r^2}$ ⇐ E FORCES

$L = n\hbar$ ⇐ ANGULAR MOMENTUM ASSUMPTION

$E_2 - E_1 = h\nu$ ⇐ DISCRETE ORBIT ASSUMPTION

SOLVING FOR E GIVES

$E_n = \frac{mZ^2e^4}{32\pi^2\epsilon^2 n^2\hbar^2}$ ⟸ ORBITAL ENERGY

$E_n - E_m = \epsilon$ = PHOTON EN. $= h\nu_{nm} = \frac{mZ^2e^4}{32\pi^2\epsilon^2\hbar^2}\left(\frac{1}{n^2} - \frac{1}{m^2}\right)$

9-8-75 (MON)

HOMEWORK: DUE MON 9-15-75

TEXT PROBLEMS 1.4, 1.5, 1.7, 1.11, 1.15

6 MAKE AN ENERGY LEVEL DIAGRAM FOR THE BOHR ATOM

NOTES: $E = h\nu = R\left(\frac{1}{n^2} - \frac{1}{m^2}\right)$ $n, m > 0$, $n, m \in$ INTEGER, $n < m$

IONIZATION ENERGY ⇒ $n = 1$, $m = \infty$

THEN $E_{MAX} = 13.6$ eV (?) = 105,000 cm^{-1} (?)

WHERE cm^{-1} IS A UNIT OF ENERGY.

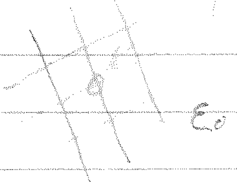
1 MICRON = 10^{-6} m (INFRARED ⇒ $.7\mu < \lambda < 500\mu$)

10,000 Å = 1μ

NOW, $E = h\nu = h\frac{c}{\lambda}$

$\frac{10,000}{\# \text{MICRONS}}$ = # OF cm^{-1}

IMPURITY (DONOR, EXTRA ELECTRON)



$E_{BIND} = 13.6\,eV \times \frac{\epsilon_0^2}{\epsilon^2} \times \frac{m^*}{m}$

$\epsilon/\epsilon_0 \cong 12$

$\Rightarrow E_{BIND} \cong 0.1$ eV

$eE = m^*a$

↑ EFFECTIVE MASS

SCHOEDINGER'S EQUATION

ENERGY EQUATION

$$(K.E. + P.E.)\, f(x) = E\, f(x) \Leftarrow \text{EIGEN VALUE FORM}$$

$$\left(\frac{p^2}{2m} + V(r)\right) f(x) = E\, f(x)$$

GIVES SCHROUDINGER'S EQN. AS

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V(r)\,\psi = E\psi$$

WILL GIVE ALLOWED ENERGY STATES IN SOLIDS

SIMPLEST SOLUTION IS FOR $V(r) = 0$

CONSIDER IN ONE DIMENSION:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi$$

$$\Rightarrow \frac{d^2\psi}{dx^2} - \left(\frac{2mE}{\hbar^2}\right)\psi = 0$$

$$\frac{d^2\psi}{dx^2} + k^2\psi = 0 \quad \Rightarrow k^2 = -\frac{2mE}{\hbar}$$

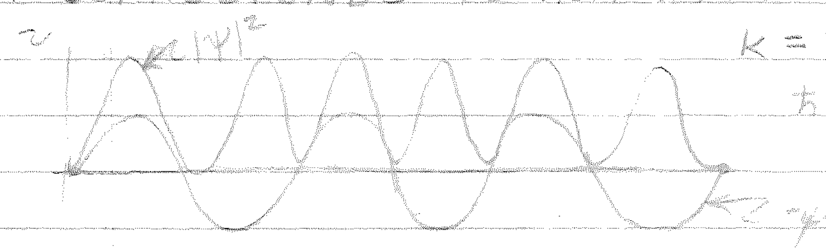
TWO SOLUTIONS:

$$\psi = Ae^{ikx} + Be^{-ikx} = A'\sin kx + B'\cos kx$$

K CORRESPONDS TO MOMENTUM $p = \hbar k$; $k = \frac{2\pi}{\lambda}$

$$k = \sqrt{\frac{2mE}{\hbar^2}}$$

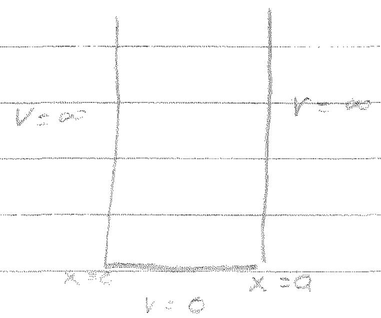
$\hbar k = \sqrt{2mE} = mv$



PROBABILITY OF THE PARTICLE BEING AT POINT $x = |\psi(x)|^2$ AND $\int_{-\infty}^{\infty} |\psi(x)|^2 dx = 1$

UNCERTAINTY PRINCIPLE: $\Delta x \Delta p \geq \hbar/2$

POTENTIAL WELL WITH INFINATE WALLS



$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V\psi = E\psi$$

FOR $V=\infty$, $\psi=0 \Rightarrow \psi=0$ FOR $x\leq 0, x\geq a$

SO BOUNDRY CONDITIONS ARE

$\psi(0)=\psi(a)=0$

$\frac{d\psi(0)}{dx} = \frac{d\psi(a)}{dx} = 0 \Leftarrow$ NOT VALID FOR ∞ WALLS

FOR $0<x<a$, $\psi(x) = A\sin kx + B\cos kx$

$\psi(0)=0 \Rightarrow B=0$

$\psi(a)=0 \Rightarrow A\sin ka = 0 \Rightarrow ka = n\pi \Rightarrow k=\frac{n\pi}{a}$

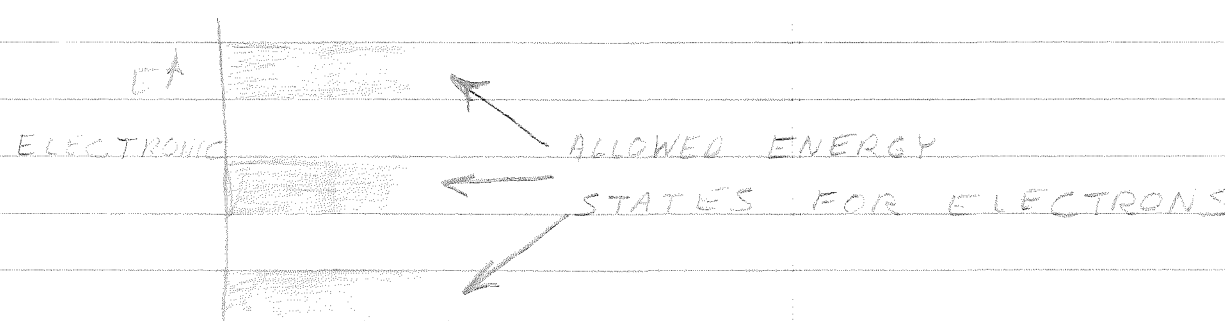
(NOTE THAT E CAN BE HERE SOLVED FOR — SPECIFICALLY, $k=\sqrt{\frac{2mE}{\hbar^2}} \Rightarrow E_n = \frac{\hbar^2 n^2\pi^2}{2ma^2}$)

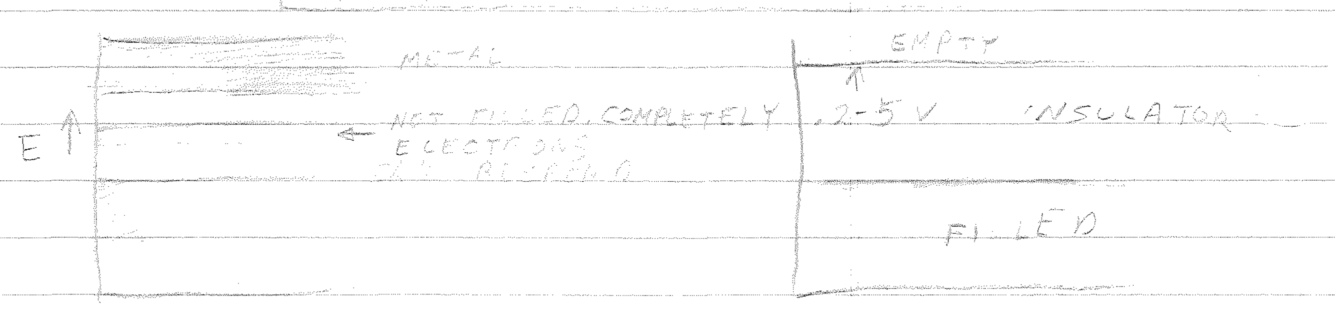
$\Rightarrow \int_0^a |A|^2 \sin^2 kx\,dx = 1$ GIVES A

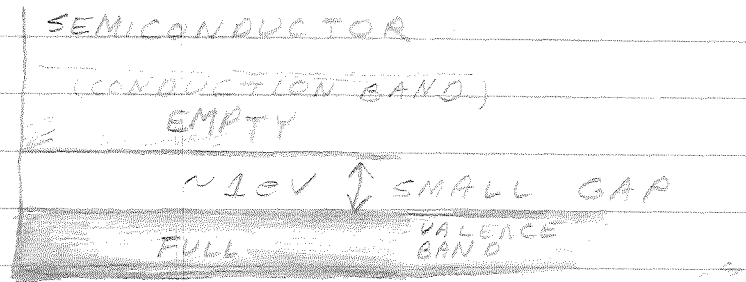
9-10-75 (WED)

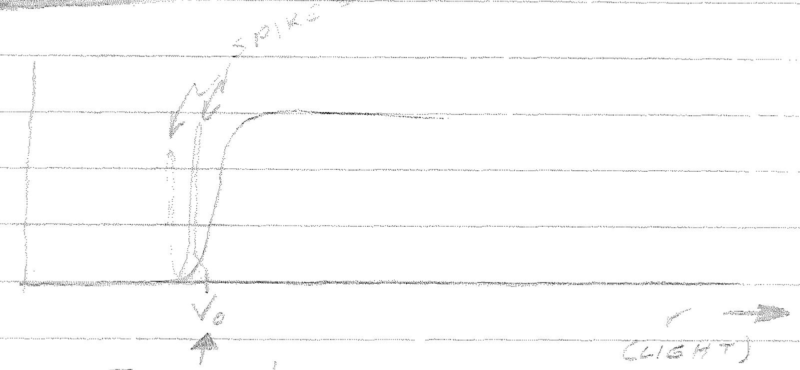
ENERGY LEVEL STRUCTURE OF A SOLID

ENERGY TYPICALLY $0.0005\,eV < E < 5\,eV$



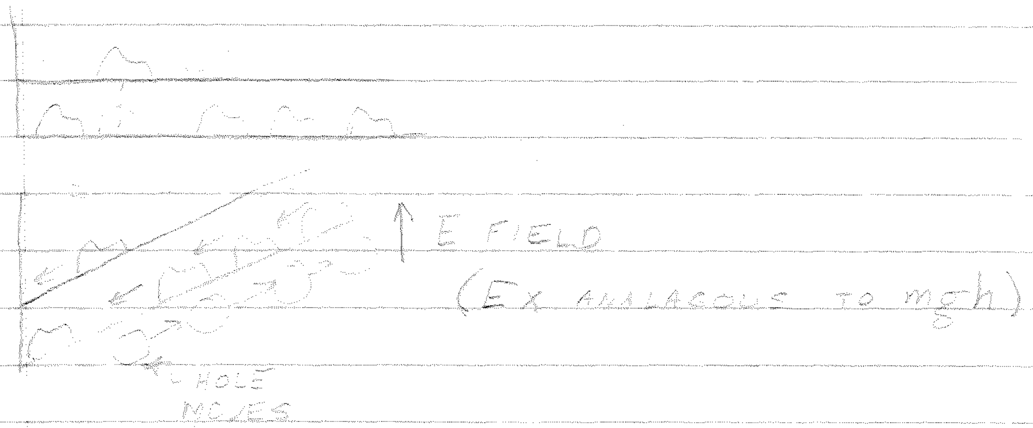




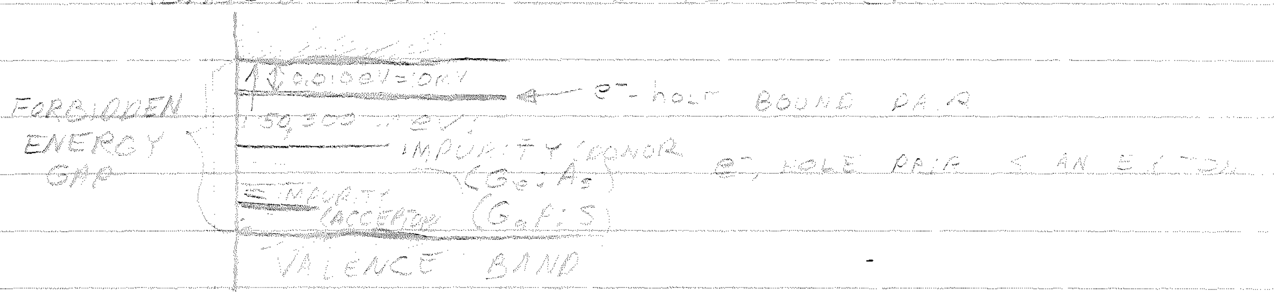


$E_{gap} = h\nu_0$

PARKING LOT EXAMPLES OF HOLES



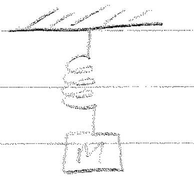
REASON FOR SPIKES IS IMPURITIES



8

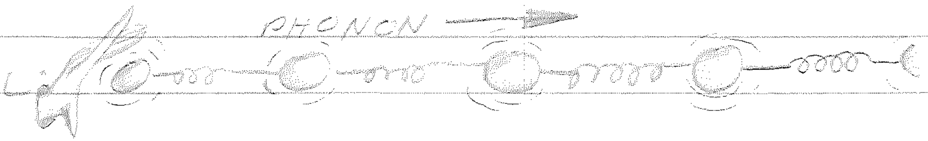
SEMICONDUCTOR CLASSES

IV - IV		II	III	IV	V	VI
III - V		Cd	Ga	Ge	P	S
II - VI		Zn	Sb	Si	As	Te
						Se



$\omega = \sqrt{K/M}$

IN CRYSTAL



9-12-75 (FRI)

SCH. EQ.N:

HARMONIC OSC.: $-\frac{\hbar^2}{2m}\nabla^2\psi + \frac{m\omega^2 x^2}{2}\psi = E\psi$

FOR HYDROGEN:

$$-\frac{\hbar^2}{2m}\nabla^2\psi - \frac{e^2}{4\pi\epsilon_0 r}\psi = E\psi$$

FOR GENERAL ATOM:

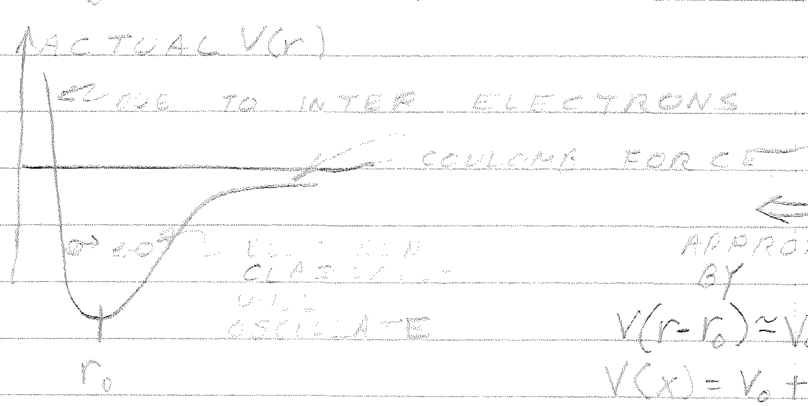
$$-\underbrace{\sum_i^N \frac{\hbar^2 \nabla_i^2}{2m}\psi}_{K.E.} - \underbrace{\sum_{i=1}^N \frac{e^2}{4\pi\epsilon_0 r_i}\psi}_{P.E.} + \frac{1}{2}\sum_{i\neq j}^N \frac{e^2}{4\pi\epsilon_0 |\vec{r}_i - \vec{r}_j|}\psi = E\psi$$

MATHEW'S EQUATION:

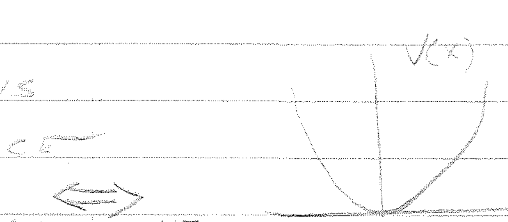
$\psi'' + (\eta + \delta \cos 2x)\psi = 0$ ← GOOD FOR PERIODIC SOLIDS

EIGEN VALUE   PERIODICITY

ONE DIMENSIONAL HARMONIC OSCILLATOR



⟺ APPROXIMATE BY



$$V(r-r_0) \simeq V_0 + r\frac{\delta V}{\delta r}\Big|_{r=r_0} + \frac{r^2}{2!}\frac{\delta^2 V}{\delta r^2}(r-r_0)$$

$$V(x) = V_0 + x\frac{\delta V}{\delta r}\Big|_{r_0} + \frac{1}{2!}\frac{\delta^2 V}{\delta r_0^2}x^2 + \dots$$

CONT →

V_0 IS A CONSTANT (NO PROBLEM TO DEFINE)

$\frac{dV}{dr}$ @ MINIMUM = 0

$\frac{1}{2!} \frac{\delta^2 V}{\delta r^2}\Big|_{r=0} x^2$; LET $m\omega^2$ = CONSTANT = $\frac{\delta^2 V}{\delta r^2}\Big|_{r=0}$

GIVES: $V(x) = \frac{1}{2} m\omega^2 x^2$

$\Rightarrow$ APPROXIMATE WELL WITH A PARABOLA

$\frac{1}{3!} \frac{\delta^3 V}{\delta r^3} x^3$ IS SOMETIMES USED

SCHRÖ'S EQ FOR HARMONIC OSC. IS

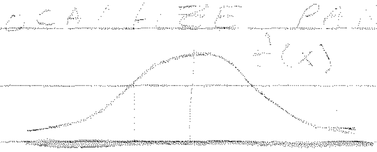
$$-\frac{\hbar^2}{2m} \frac{\delta^2}{\delta x^2} \psi + \frac{1}{2} m\omega^2 x^2 \psi = E\psi$$

9-17-75 (WED) READ CHAPT 2 UP TO 2.5

PHASE VELOCITY $\rightarrow \frac{\omega}{k} = \nu\lambda \Rightarrow \omega = 2\pi\nu, \; k = \frac{2\pi}{\lambda}$

GROUP VELOCITY

LOCALIZE PARTICLE

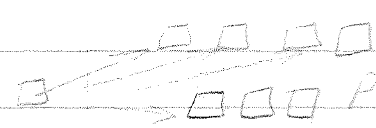


$f(x) = \sum a_k e^{ikx}$

GROUP VELOCITY = PARTICLE VELOCITY = $\frac{d\omega}{dk}$

FERMI ENERGY = f(# electrons, TEMP, IMPURITIES)

PAULI EXCLUSION PRINCIPLE



(EQUIVALENT # OF STATES)

$\rho(E)$ = DENSITY OF STATES (AS A FUNCTION OF ENERGY

RATE OF TRANSITION = $\frac{2\pi}{\hbar} \left| \int \psi_f V \psi_i \right|^2 \rho(E)$

10.

EFFECTIVE MASS OF A CRYSTAL

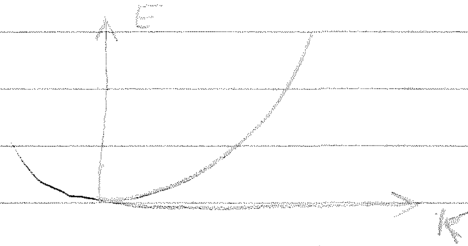
$p = \hbar k$

$E = \hbar \omega$

$F = ma = \frac{dp}{dt} = qE$

$E = p^2/2m$

$= \frac{\hbar^2 k^2}{2m^*}$



DISPERSION CURVES

$F = \frac{dp}{dt} = \hbar \frac{dk}{dt} = m^* \frac{dv_g}{dt} = m^* \frac{d}{dt}\frac{d\omega}{dk}$

$\hbar^2 \frac{dk}{dt} = m^* \frac{d}{dt}\left(\frac{d\hbar\omega}{dk}\right)$

$= m^* \frac{d}{dk}\frac{dE}{dk}\left(\frac{dk}{dt}\right)$

IN 3-d:

$$m^*_{ij} = \frac{\hbar^2}{\frac{\delta^2 E}{\delta k_i \delta k_j}}$$

THUS, EFFECTIVE MASS IS RELATED TO <u>INTRINSIC</u> CRYSTAL PROPERTIES

HARMONIC OSCILLATOR: SOLUTION

$-\frac{\hbar^2}{2m}\frac{\delta^2\psi}{\delta x^2} + \frac{1}{2} m\omega^2 x^2 \psi = E\psi$

$\frac{\delta^2\psi}{\delta\xi^2} + (E - \gamma\xi^2)\psi = 0$

$\psi = e^{-\xi^2} U(\xi)$

ASSUME SOLUTION $U = \sum a_n \xi^n$

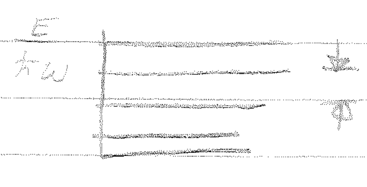
END UP WITH $\sum(\alpha a_n + \beta a_{n+2})\xi_n = 0$

$U(\xi) = a_0 \sum_n \alpha(n)\xi^n$

GET a_0 BY NORMALIZATION

SOLUTION IS HERMITE POLYNOMIALS

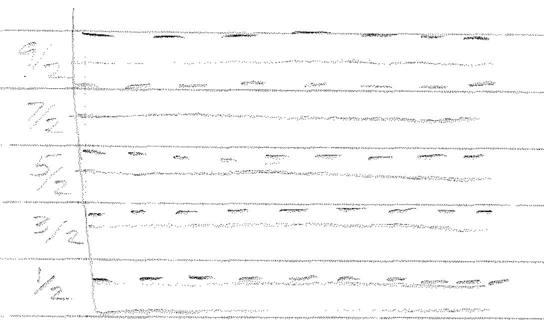
TURNS OUT $E_n = (n + \frac{1}{2})\hbar\omega$



FROM $V = \frac{1}{2}\gamma X^2$

FOR $V = \frac{1}{2}\gamma x^2 + \text{CONST } x^3$ (- - - -)

HARMON. OSC. (——)



9-19-75 (FRI)

WAVE PROPAGATION IN PERIODIC STRUCTURES

by L. BRILLOUIN (DOVER PAPERBACK)

BRILLOUIN ZONE

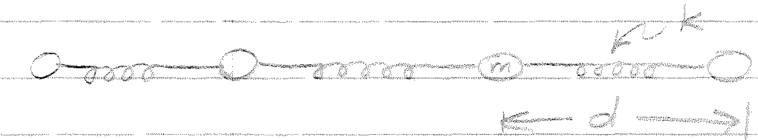
PROBLEMS OF WHICH THE BZ IS AN ASPECT

① PHONON (SOUND - LATTICE VIBRATIONS) STRUCTURE OF A SOLID

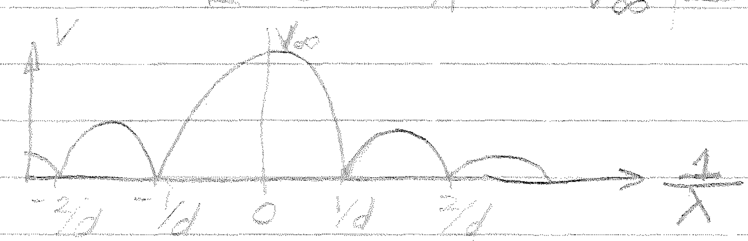
② ELECTRONIC ENERGY STRUCTURE

LAGRANGE (1759)

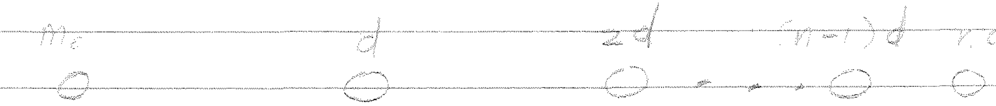
PROPER FUNCTIONS



V = VELOCITY $= V_\infty \left| \frac{\sin \pi d/\lambda}{\pi d/\lambda} \right|$



TRANSVERSE DISPLACEMENT



Y_n = DISPLACEMENT OF n^{th} MASS

$= A \cos(\omega t - knd)$

$k = \frac{2\pi}{\lambda}$, A = CONSTANT

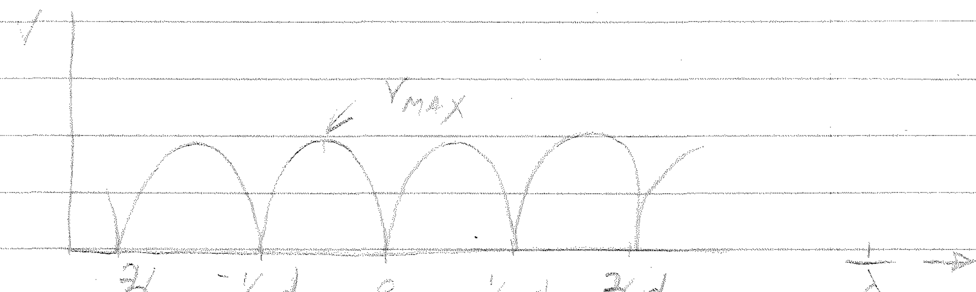
REPLACE k BY $k + \frac{2\pi n}{d}$ GIVES

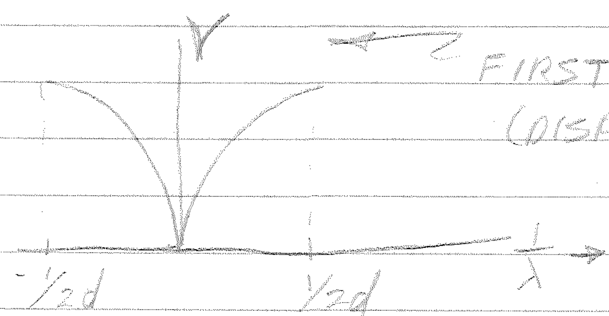
THE SAME THING

$k = \frac{2\pi}{\lambda} \Leftrightarrow \frac{2\pi}{\lambda} + \frac{2\pi n}{d}$

(POOT OF BRILLUON ZONE)

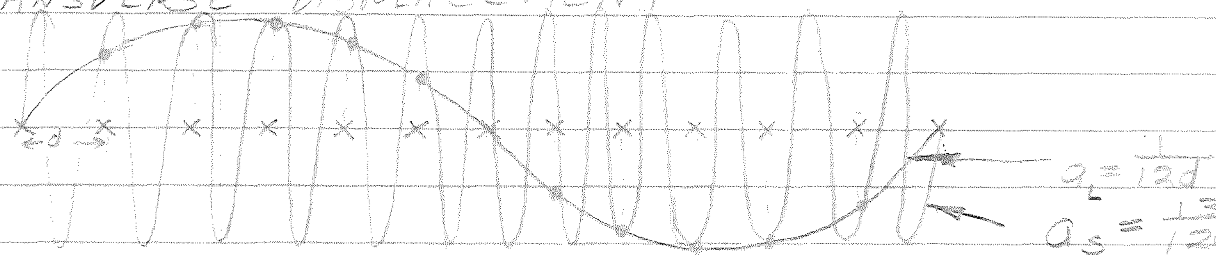
$\nu = \nu(a = \frac{1}{\lambda}) = \text{CONST} \left| \sin \pi a d \right|$





FIRST BRILLOUIN ZONE
(DISPERSION CURVE)

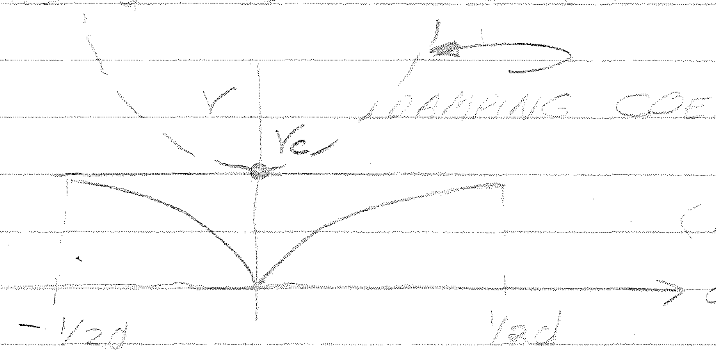
TRANSVERSE DISPLACEMENT



$\frac{13}{12}d = \frac{1}{12d} + \frac{1}{d}$ ⇒ INTEGRAL ADDITION OF $\frac{1}{d}$

∴ MAY RESTRICT $-\frac{1}{2d} < a = \frac{1}{\lambda} \leq \frac{1}{2d}$

AS $d \to \infty$ $\quad -\infty < a < \infty$ (AS IN A STRING)

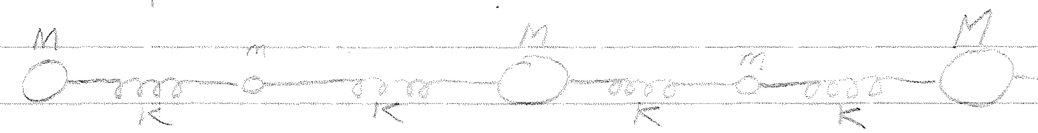


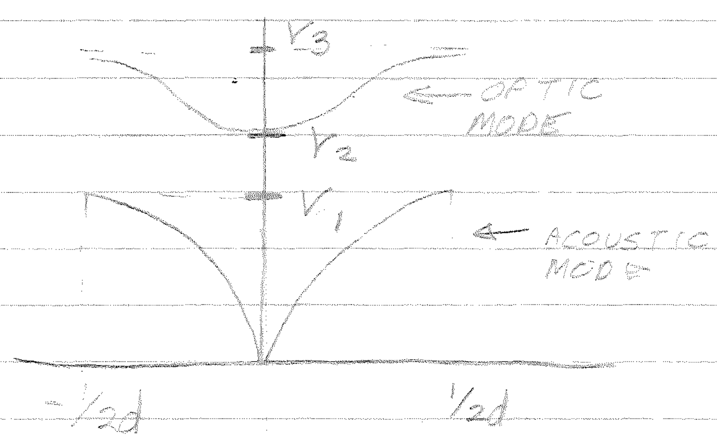
DAMPING COEFFICIENT β

ATTENUATION $\nu > \nu_c$

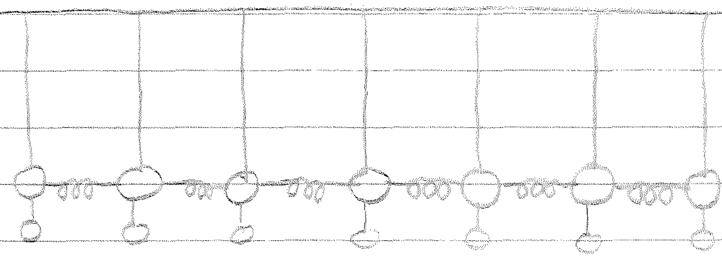
(AKIN TO LO-PASS FILTER)

FOR UNEQUAL MASSES:

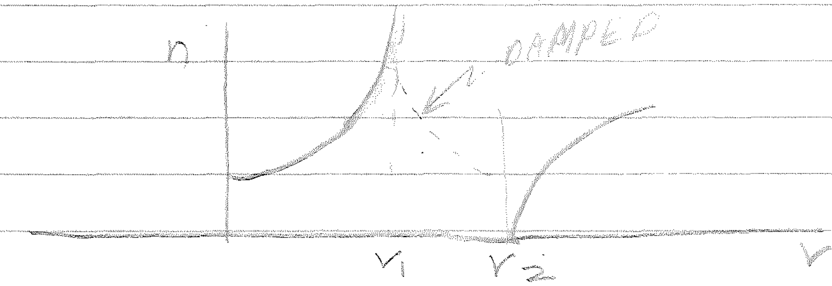




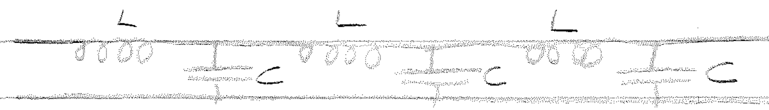
DISPERSION CURVE



← WILL HAVE STOP BAND.



FOR THE ONE MASS CASE:

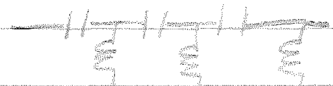


$$\nu_c = \frac{1}{\pi\sqrt{2LC}}$$

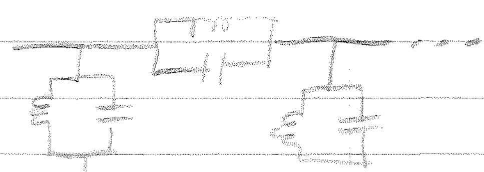
9-22-75 (MON)

COULD HAVE

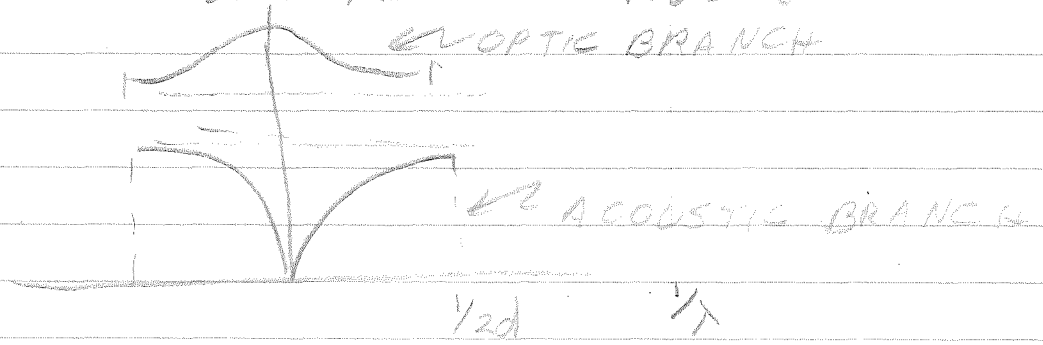
HI PASS



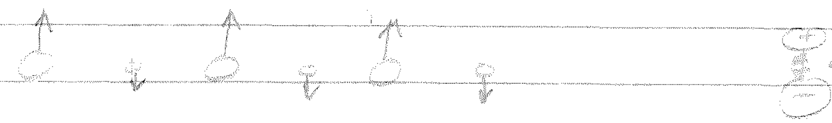
BAND PASS ...



DIATONIC DISPERSION CURVE (PERIODIC)

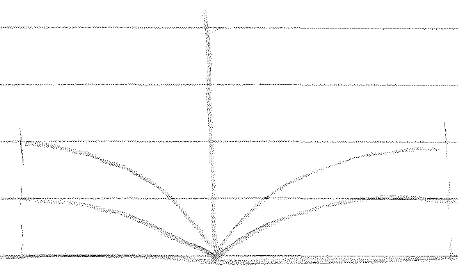


OPTIC BRANCH (PRODUCES DIPOLE MOMENT)



$\omega = \sqrt{K/M}$

TWO TRANSVERSE AND TWO LONG. MODES



1 LONG. ⇒ DIRECTION OF PROPAGATION
2 TRAN ⇒ NORMAL TO LONGITUDINAL

LATTICE SPACING: $nd + Y_n$

$$Y_n = A e^{i(\omega t - nkd)} \qquad > k = \frac{2\pi}{\lambda}$$

ν = FREQUENCY, $\omega = 2\pi\nu$, λ = WAVELENGTH

t = TIME, d = LATTICE SPACING

n = INTEGER, A = CONSTANT AMPLITUDE

$k = \frac{2\pi}{\lambda}$, $a = 1/\lambda$

$$Y_{n+1} = e^{-ikd}\, Y_n$$

$k' = k + 2\pi n/d$ ⇐ MAY REDUCE TO 1ST ZONE

ω IS PERIODIC IN kd

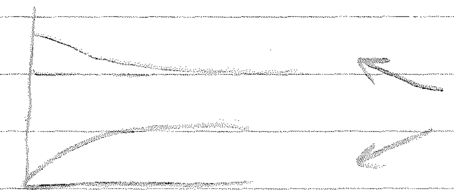
LET $-\frac{1}{2d} \leq a < \frac{1}{2d}$ OR $-\frac{\pi}{d} \leq k < \frac{\pi}{d}$

(NEGATIVE WAVE #'S: $k > 0$ ⇒ WAVE PROPAGATING TO THE RIGHT, $k < 0$ TO THE LEFT)

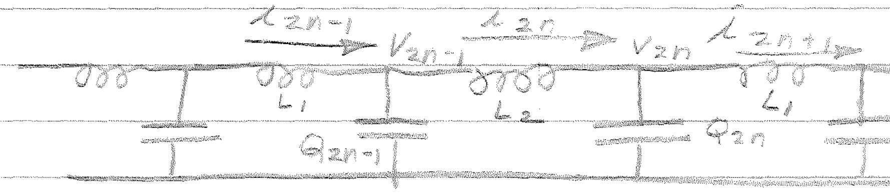
$f(\lambda)$ = EVEN FUNCTIONS

IF FOR EACH k, $\exists$ N DEGREES OF FREEDOM, THEN THERE ARE K BRANCHES.

1-D LATTICE, 2 ATOMS PER CELL:



PROBLEM:



$$i_{2n} - i_{2n+1} = \frac{d}{dt} Q_{2n}$$
$$i_{2n+1} - i_{2n+2} = \frac{d}{dt} Q_{2n+1}$$

$$L_1 \frac{d i_{2n+1}}{dt} = \frac{Q_{2n}}{C_1} - \frac{Q_{2n+1}}{C_2}$$
$$L_2 \frac{d i_{2n}}{dt} = \frac{Q_{2n-1}}{C_2} - \frac{Q_{2n}}{C_1}$$

GET TWO SECOND ORDER EQUATIONS:

$$\begin{cases} L_1 \dfrac{d^2 i_{2n+1}}{dt^2} = \dfrac{i_{2n} - i_{2n+1}}{C_1} - \dfrac{i_{2n+1} - i_{2n+2}}{C_2} \\[2ex] L_2 \dfrac{d^2 i_{2n}}{dt^2} = \dfrac{i_{2n-1} - i_{2n}}{C_2} - \dfrac{i_{2n} - i_{2n+1}}{C_1} \end{cases}$$

USE $i_{2n} = A_2 e^{i(\omega t - 2nk_1 x)}$

$i_{2n+1} = A_1 e^{i[\omega t - (2n+1)kx]}$

PLUGGING BACK IN GIVES

$$\left(-L_1\omega^2 + \frac{1}{C_1} + \frac{1}{C_2}\right)A_1 - \left(\frac{e^{ikx}}{C_1} + \frac{e^{-ikx}}{C_2}\right)A_2 = 0$$

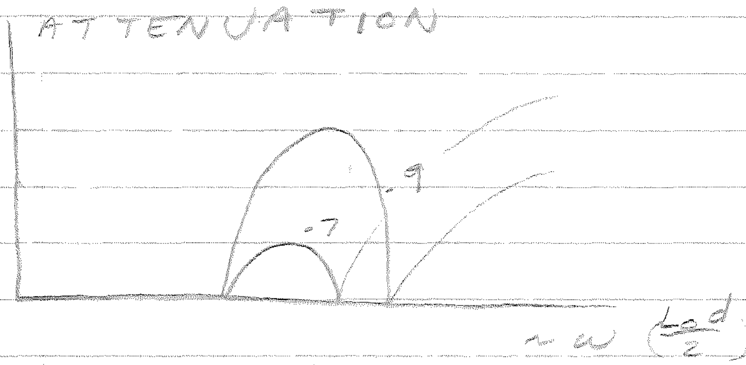
$$\left(L_2\omega^2 + \frac{1}{C_1} + \frac{1}{C_2}\right)A^2 - \left(\frac{e^{ikx}}{C_2} + \frac{e^{-ikx}}{C_1}\right)A_1 = 0$$

FOR A SOLUTION TO EXIST, det | | = 0

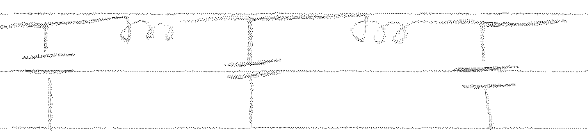
$$\left[-L_1\omega^2 + \frac{1}{C_1} + \frac{1}{C_2}\right]\left[-L_2\omega^2 + \frac{1}{C_1} + \frac{1}{C_2}\right] - \left(\frac{e^{ikx}}{C_1} + \frac{e^{-ikx}}{C_2}\right)\left(\frac{e^{ikx}}{C_2} + \frac{e^{-ikx}}{C_1}\right) = 0$$

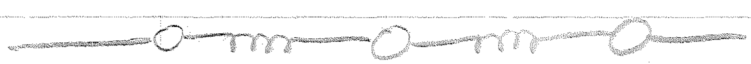
$$\omega^4 - \omega^2\left(\frac{1}{L_1} + \frac{1}{L_2}\right)\left(\frac{1}{C_1} + \frac{1}{C_2}\right) + \frac{4\sin^2 kx}{L_1 L_2 C_1 C_2} = 0$$

$$\Rightarrow \omega = \frac{1}{2}\left(\frac{1}{L_1} + \frac{1}{L_2}\right)\left(\frac{1}{C_1} + \frac{1}{C_2}\right) \pm \sqrt{\frac{1}{4}\left(\frac{1}{L_1} + \frac{1}{L_2}\right)^2\left(\frac{1}{C_1} + \frac{1}{C_2}\right) - \frac{4\sin^2 kx}{L_1 L_2 C_1 C_2}}$$



$L_1 = mL_0$





$U_{nm} = U(|X_{n+m} - X_n|) \Rightarrow$ POTENTIAL ENERGY

$U_{TOTAL} = \sum_{n,m} U(|X_{n+m} - X_n|) \Leftarrow$ NOW, MAKE AN EXPANSION

$$U(|X_{n+m} - X_n|) \sim U(md) + (Y_{n+m} - Y_n)\,U'(md) + \frac{1}{2}(Y_{n+m} - Y_n)^2\,U''(md) + \cdots$$

18

9-24-75 (WED.)

REVIEW:

DEVELOPING DISPERSION CURVE FOR 1-D LATTICE:

$$\cdots \overset{M_2}{\underset{2n-1}{C}} \quad \overset{M_1}{\underset{2n}{C}} \quad \overset{M_2}{\underset{2n+1}{C}} \quad \overset{M_1}{C}$$

$$\underbrace{X_{n+m} \qquad X_n}$$

$$U[|X_{n+m} - X_n|] = U_{md} + (Y_{n+m} - Y_n)\,U'(md) + \tfrac{1}{2}(Y_{n+m} - Y_n)^2\,U''(md) + \ldots$$

$$U \doteq \sum_n \sum_{m>0} \left[U(md) + (Y_{n+m} - Y_n)\,U'(md) + \tfrac{1}{2}(Y_{n+m} - Y_n)^2\,U''(md) \right]$$

$$F_p = -\frac{\delta U}{\delta Y_p} = -\frac{d}{dY} \sum_{m>0} \left[(Y_{p+m} - Y_p)\,U'(md) + \tfrac{1}{2}(Y_{p+m} - Y_p)^2\,U''(md) + (Y_p - Y_{p-m})\,U'(md) + \tfrac{1}{2}(Y_p - Y_{p-m})^2\,U''(md) \right]$$

$$= -\sum_{m>0} \left[-U'(md) - (Y_{p+m} - Y_p)\,U''(md) + (Y_p - Y_{p-m})\,U''(md) + U'(md) \right]$$

$$= \sum_{m>0} U''(md) \left[Y_{p+m} + Y_{p-m} - 2Y_p \right]$$

IGNORING HIGHER TERMS:

$$\begin{cases} F_{2n} = U_1''(Y_{2n-1} + Y_{2n+1} - 2Y_{2n}) = M_2 \dfrac{d^2 Y_{2n}}{dt^2} \\ F_{2n+1} = U_1''(Y_{2n} + Y_{2n+2} - 2Y_{2n+1}) = M_1 \dfrac{d^2 Y_{2n+1}}{dt^2} \end{cases}$$

ASSUME SOLUTION FORMS:

$$Y_{2n} = A_2 e^{i(\omega t - nkd)} \quad ; \; k = \frac{2\pi}{\lambda}$$

$$Y_{2n+1} = A_1 e^{i(\omega t - \frac{2n+1}{2}kd)}$$

PLUGGING IN GIVES

$$\begin{cases} M_2(-A_2\omega^2) = U_1''\left[A_1 e^{i\frac{kd}{2}} + A_1 e^{-i\frac{kd}{2}} - 2A_2\right] \\ M_1(-A_1\omega^2) = U_1''\left[A_2 e^{i\frac{kd}{2}} + A_2 e^{-i\frac{kd}{2}} - 2A_1\right] \end{cases}$$

OR

$$\begin{cases} A_2(M_2\omega^2 - 2U_1'') + 2A_1 U_1'' \cos\frac{kd}{2} = 0 \\ A_1(M_1\omega^2 - 2U_1'') + 2A_2 U_1'' \cos\frac{kd}{2} = 0 \end{cases}$$

TAKE A LOOK NOW OF THE DET. OF COEFFICIENTS.

REQUIRE $\det(\;) = 0$

$$\Rightarrow \omega^4 - 2U_1''\left(\frac{1}{M_1} + \frac{1}{M_2}\right)\omega^2 + \frac{4U_1''^2}{M_1 M_2}\sin^2\left(\frac{kd}{2}\right) = 0$$

GIVES:

$$\Rightarrow \omega^2 = U_1''\left[\left(\frac{1}{M_1} + \frac{1}{M_2}\right) \pm \sqrt{\left(\frac{1}{M_1} + \frac{1}{M_2}\right)^2 - \frac{4\sin^2\left(\frac{kd}{2}\right)}{M_1 M_2}}\right]$$

PROBLEM: ANALYZE THE CASE $M_1 = M_2$.
FIND THE VELOCITY OF A PROPAGATING WAVE
TURN IN NEXT TUESDAY $v(k)$

NOW: $\omega^2 = \frac{U_1''}{M_1 M_2}\left[M_1 + M_2 \pm \sqrt{M_1^2 + M_2^2 + 2M_1M_2\cos kd}\right]$

ASSUME THAT $M_1 > M_2$ FOR LONG WAVELENGTHS ($\lambda >> d$) AND $k << \frac{1}{d}$

$$\Rightarrow \cos kd \cong 1 - \frac{k^2 d^2}{2} \Rightarrow \sqrt{\;\;} \cong M_1 M_2\left[1 - \frac{k^2 d^2}{2}\frac{M_1 M_2}{(M_1 + M_2)}\right]$$

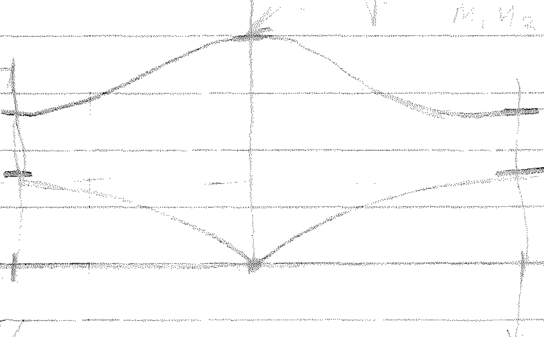
$$\omega_- = kd\sqrt{\frac{U_1''}{2(M_1 + M_2)}}$$

$$\sqrt{\frac{2U_1''(M_1 + M_2)}{M_1 M_2}}$$

$$\omega_+ = \sqrt{2U_1''\left(\frac{1}{M_1} + \frac{1}{M_2} - \frac{k^2 d^2}{4(M_1 + M_2)}\right)}$$

$\omega_+ = \sqrt{\frac{2U_1''}{M_1}}$

$\omega_- = \sqrt{\frac{2U_1''}{M_2}}$



$-\pi/d$ $\qquad$ π/d

OUT OF PHASE: $\left.\frac{A_1}{A_2}\right|_+ = 1 + \frac{k^2 d^2}{8}\left(\frac{M_1 - M_2}{M_1 + M_2}\right)$

IN PHASE: $\left.\frac{A_1}{A_2}\right|_- = -\frac{M_2}{M_1}\left[1 - \frac{k^2 d^2}{8}\frac{(M_1 - M_2)}{(M_1 + M_2)}\right]$

AT ZONE BOUNDARY, $\cos kd \cong -\cos(\epsilon) \cong \epsilon \ldots$
$\cong 1 + \frac{\epsilon^2}{2}$

$$\sqrt{\;\;} \cong (M_1 - M_2)\left[1 + \frac{\epsilon^2 M_1 M_2}{2(M_1 - M_2)}\right]$$

$$\omega_+ = \sqrt{U_1''\left(\frac{2}{M_2} + \frac{\epsilon^2}{2(M_1 - M_2)}\right)}$$

$$\omega_- = \sqrt{U_1''\left(\frac{2}{M_1} - \frac{\epsilon^2}{2(M_1 - M_2)}\right)}$$

DISPERSION

1. $\omega^2\left(\frac{M_1+M_2}{2U_1}\right) - \frac{\omega^2 M_1 M_2}{4U_1^2} = \sin^2\frac{kd}{2} > 1$

TO INCLUDE FORBIDDEN ZONE MUST EMPLOY IMAGINARY ARGUMENTS.

2. $kd = \alpha + i\beta$, THEN

$$\sin\frac{kd}{2} = \sin\frac{\alpha}{2}\cosh\frac{\beta}{2} + i\cos\frac{\alpha}{2}\sinh\frac{\beta}{2}$$

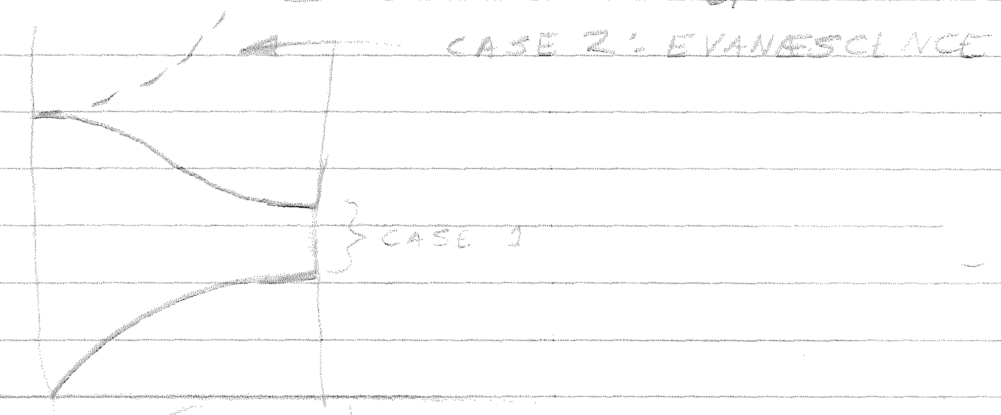
$$\frac{\alpha}{2} = \frac{\pi}{2}$$

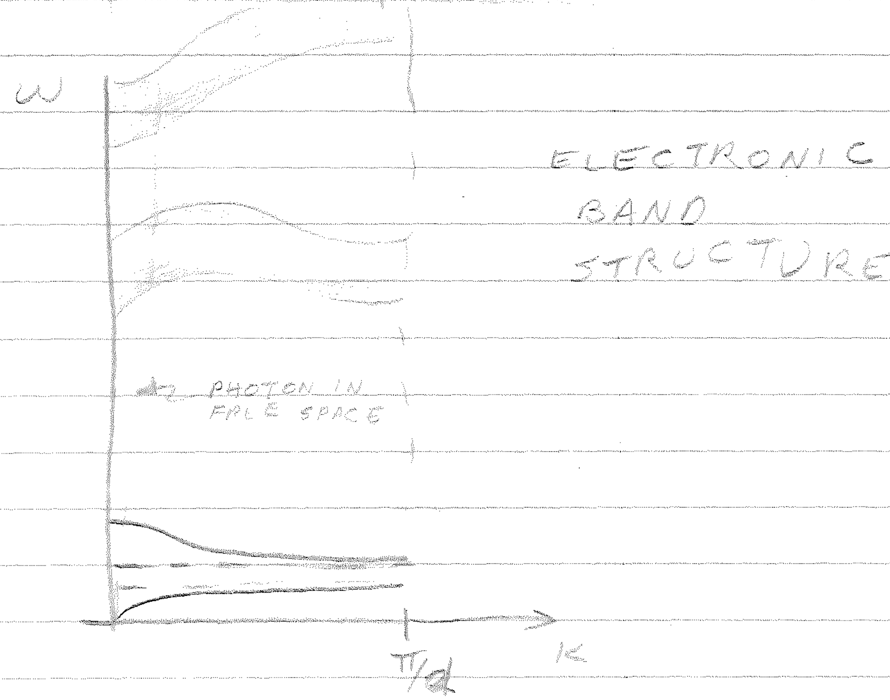
$\omega^2 < 0 \Rightarrow \operatorname{Im}\omega$

$\Rightarrow \operatorname{Re}\sin\frac{kd}{2} = 0$

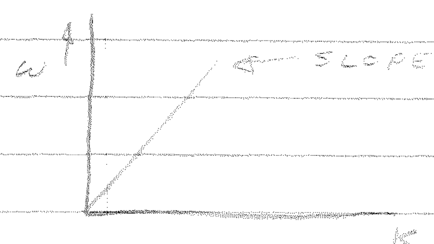
$\sin\frac{\alpha}{2}\cos\frac{\beta}{2} = 0$

$\Rightarrow \frac{\alpha}{2} = 0 \Rightarrow k = \frac{i\beta}{d}$





PHOTON IN FREE SPACE



$\omega = CK$

DUE WED.

② WHAT IS K AT THE BRILLOUIN ZONE BOUNDARY FOR $d = \frac{1}{2}$ Å IN cm^{-1}? (FOR A PHONON). WHAT IS K FOR A 50 meV LIGHT WAVE? FOR 3 eV?

9-26-75 (FRI)

$$i\hbar \frac{\delta \psi}{\delta t} = H\psi = E_n \psi$$

ADD A PERTURBATION $\Rightarrow i\hbar \frac{\delta \psi}{\delta t} = (H+V)\psi$

WITHOUT PERTURBATION, $\psi = \sum_n a_n \phi_n(x) e^{-i\frac{E_n t}{\hbar}}$

ASSUME, FOR PERTURBATION $a_n = a_n(t, x)$

PLUG INTO PERTURBED WAVE EQN.

$$i\hbar \left[\sum_n \frac{\delta a_n}{\delta t} \phi_n(x) e^{-i\frac{E_n t}{\hbar}} - \frac{i}{\hbar} E_n a_n \phi_n e^{-i\frac{E_n t}{\hbar}} \right]$$
$$= [H+V] \sum_n a_n \phi_n(x) e^{-iE_n t/\hbar}$$

MULTIPLY BOTH SIDES BY $\phi_n^*(x)$ AND INTEGRATE

$$i\hbar \frac{\delta a_s}{\delta t} e^{-i\frac{E_s t}{\hbar}} \cancel{+ E_s a_s e^{-i\frac{E_s t}{\hbar}}}$$
$$= \cancel{E_s a_s e^{-iE_s t/\hbar}} + \sum_n a_n \int \phi_s^* V \phi_n e^{-i\frac{E_n t}{\hbar}} dx$$

OR

$$\frac{\delta a_s}{\delta t} = -\frac{i}{\hbar} \sum_n a_n V_{sn} e^{\frac{i}{\hbar}(E_s - E_n)t}$$

$$V_{sn} = \int \phi_s^* V \phi_n \, dx$$

$$\frac{\delta a_s}{\delta t} = -\frac{i}{\hbar}\sum_n a_n V_{sn} e^{\frac{i}{\hbar}(E_s - E_n)t}$$

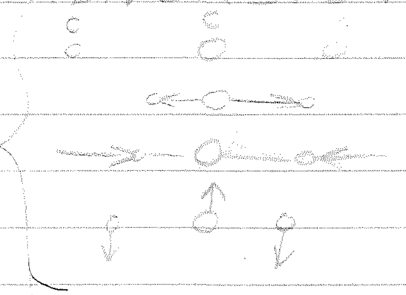
RECALL

$$\int \phi_s^* H \phi_n = E_n \delta_{sn}$$

$\int \phi_s^* V_{sn} \phi_n$ — A COUPLING TYPE NUMBER

CONVERSION

$\leftarrow CO_2$



FERMI RESONANCE

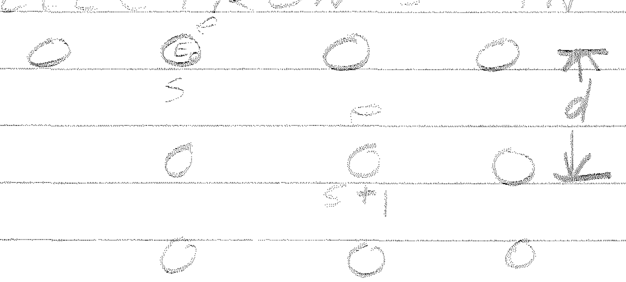
USUALLY MEASURE V_{SN} -

CONSIDER THE SPECIAL CASE WHERE —

$$E_s = E_n \Rightarrow \frac{\delta a_s}{\delta t} = -\frac{i}{\hbar}\sum_n a_n V_{sn}$$

(SEE VOL. 3 OF FEYNMANN LECTURES).

ELECTRONS IN A SOLID



ASSUME $a = e^{-i\omega t}$

$$\Rightarrow \hbar\omega a_s = \sum_n a_n V_{sn}$$

$$E a_s = \sum_n a_n V_{sn}$$

$E_0 = V_{ss}$

$$E a_s = E_0 a_s + V_{s,s+1} a_{s+1} + V_{s,s-1} a_{s-1}$$
$$+ V_{s,s+2} a_2 + V_{s,s-2} a_{s-2} + \dots$$

ASSUME ELECTRON WILL JUMP ONLY TO AN ADJACENT ATOM - THIS GIVES

$$E a_s = E_0 a_s - V_{s,s+1} a_{s+1} - V_{ss-1}$$

THUS

$(E-E_0)a_s = -V(a_{s-1} + a_{s+1})$

LET

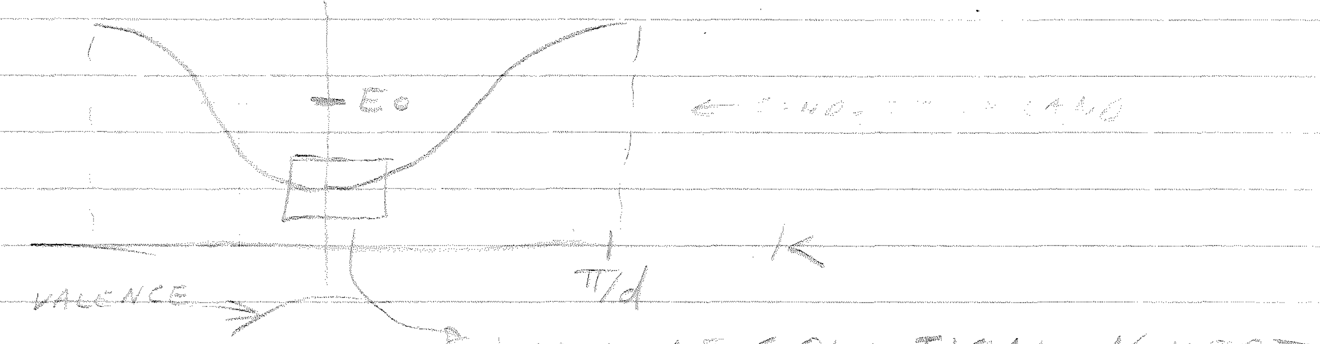
$a_{s+n} = e^{ikn d} \Rightarrow a_{s-n} = e^{-iknd}$

GIVES

$E - E_0 = -V_1\left[e^{ikd} + e^{-ikd}\right]$
$= -2V_1 \cos kd$

$$\underline{\Rightarrow E = E_0 - 2V_1 \cos kd}$$

GRAPH IT'S DISPERSION CURVE



$\cos kd = 1 - K^2 d^2/2$

$\Rightarrow E = E_0 - 2V_1 + V_1 d^2 K^2 \Leftarrow$ PARABOLA

RECALL FROM ELECTRON IN FREE SPACE: $E = \frac{\hbar^2 k^2}{2m}$, $m = \frac{\hbar^2}{2V_1 d^2} \Rightarrow$ EFFECTIVE MASS

$(E-E_0) = -V_1 2 \cos kd + V_2 2 \cos 2kd$

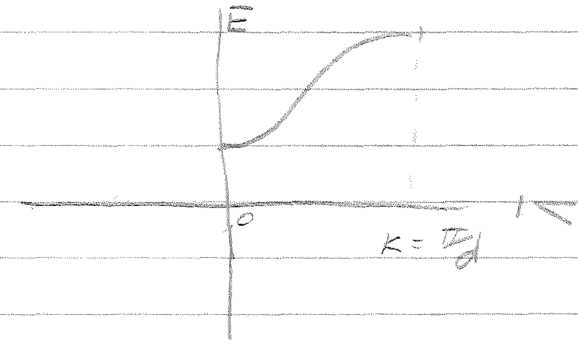
FROM USING $V_{s,s-2}\, a_{s-2} + V_{s,s+2}\, a_{s+2}$
THROWN AWAY PREVIOUSLY

9-29-75 (MON)

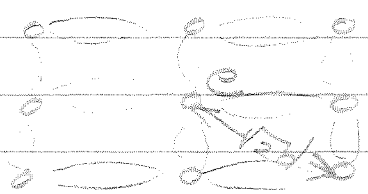
$$i\hbar \frac{\delta a_s}{\delta t} = E_0 a_s + \sum_{n=1,2,\dots} V_{s+n}\, a_{s+n}$$

ASSUMED $a = e^{ikx_n}$

GIVES $E = E_0 - 2V_1 \cos kd$

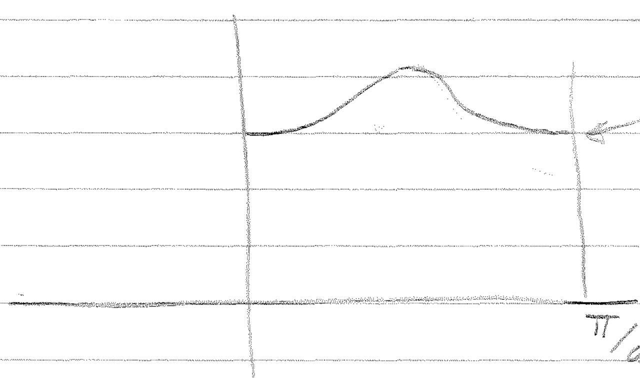


CONSIDER 2-D SOLID



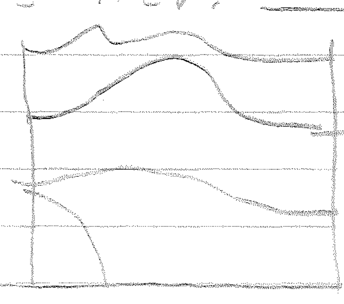
4 - V_1 TERMS

GIVES $E = E_0 - 2V_1 \cos kd + 2V_2 \cos k\sqrt{2}\, d$



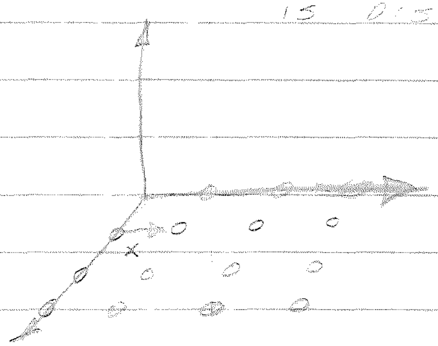
← can BE LESS THAN @ k = 0

SEE: M.L. COHEN AND K. BERGSTRESER
PHYS REV. 141, 789 (1966)



← GALLIUM PHOSPHIDES

MILLER INDICES (TO SPECIFY DIRECTIONS)

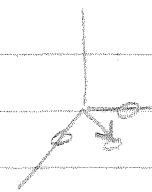


IS DISTANCE TO A PLANE

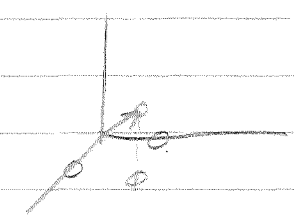
(x y z)

X $(1,0,0) = \left(\frac{1}{1}, \frac{1}{\infty}, \frac{1}{\infty}\right)$

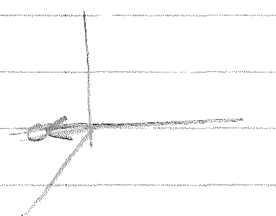
$\Rightarrow$ DISTANCE TO NEXT PLANE



$\left(\frac{1}{1}, \frac{1}{1}, \frac{1}{\infty}\right) = (1,1,0) - L$



$(1,1,1)$ Σ

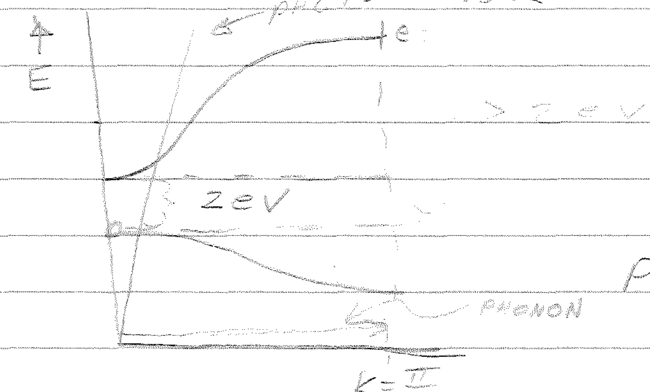


$(\bar{1},0,0)$

GOING BACKWARDS

G.F KOSTER "SPACE GROUPS AND THEIR REPRESENTATIONS", AC. PRESS

$$e_{CB} + h_{VB} \rightarrow (e,h)_{VB} + h\nu_{(E_{CB}-E_{VB})}$$

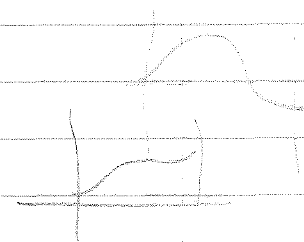


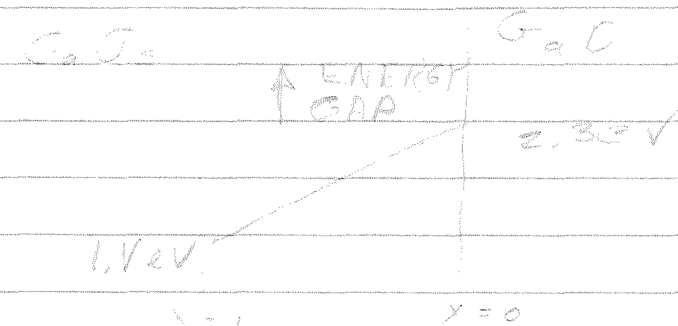
$P = \hbar K$

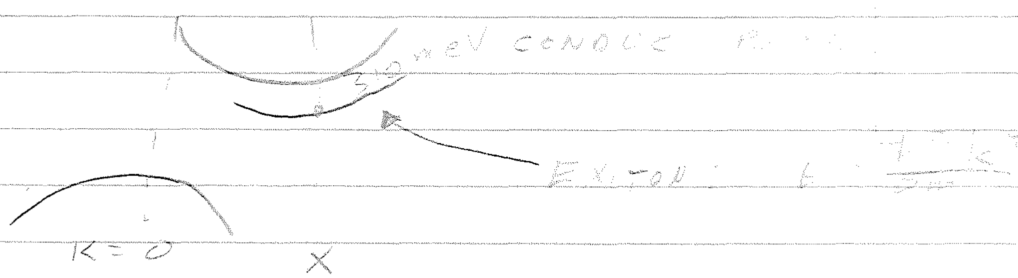
MOMENTUM CONSERVATION: $\vec{k}_e + \vec{k}_h \rightarrow 0 + \vec{k}_{h\nu}$ (PHOTON)

INDIRECT GAP (GaP)

DIRECT GAP (GaAs)





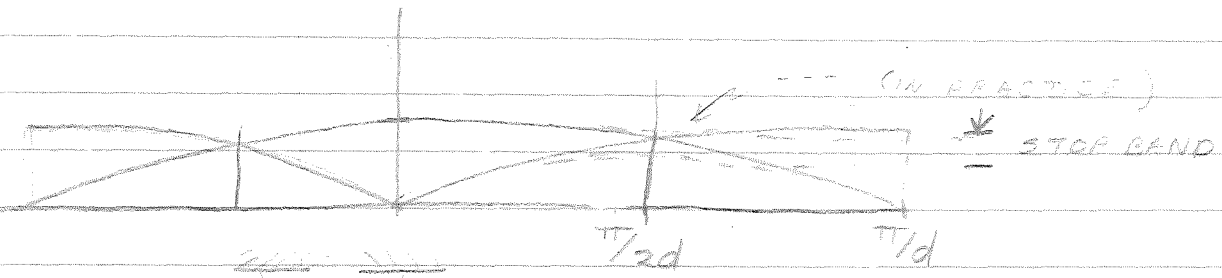


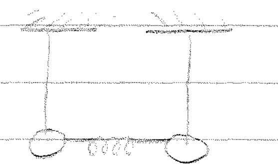
10-1-75 (WED)

ON HOMEWORK

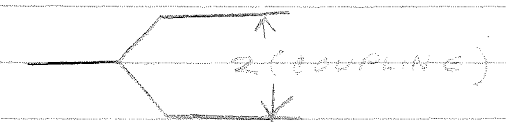
FIRST PROBLEM

GET $\omega \approx \sin\frac{kd}{2}$ AND $\omega \sim \cos\frac{kd}{2}$





$\omega = \sqrt{g/l}$



EFFECTIVE MASS

$V_g = \frac{d\omega}{dk}$; $k = \frac{2\pi}{\lambda}$

ACCELERATION OF $e = F/m^* = \frac{dV_g}{dt}$

$\left(E = \hbar\omega \Rightarrow V_g = \frac{1}{\hbar}\frac{\delta E}{\delta k} \Rightarrow V_g = \frac{1}{\hbar}\frac{\delta E}{\delta k} \right)$

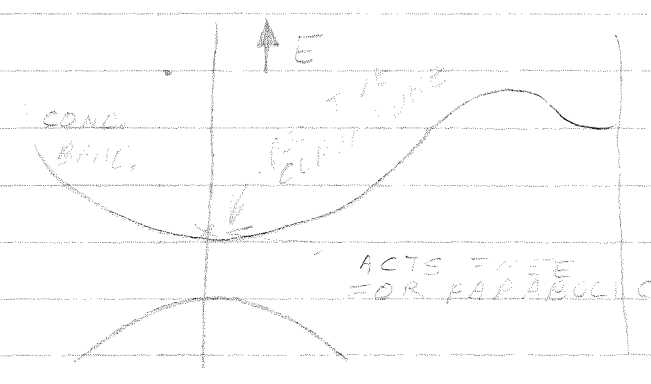
THUS ACCEL $= \frac{d}{dt}V_g = \frac{\delta}{\delta k}V_g\frac{dk}{dt} = \frac{1}{\hbar}\frac{\delta^2 E}{\delta k^2}\frac{\delta k}{\delta t}$

$p = \hbar k$

$F = \frac{dp}{dt} = \hbar\frac{dk}{dt} = m^* a$

$\frac{\hbar}{m^*}\frac{dk}{dt} = \frac{1}{\hbar}\frac{\delta^2 E}{\delta k^2}\frac{\delta k}{\delta t}$

$$\Rightarrow \boxed{m^* = \hbar^2 \Big/ \frac{\delta^2 E}{\delta k^2}}$$



$E = \frac{1}{2}mv^2$

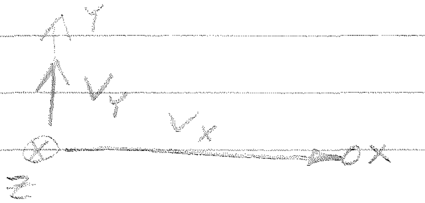
$= \frac{1}{2}\hbar^2 k^2/m$

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

PARABOLIC BAND $\Leftrightarrow$ QUASI FREE ELECTRON

PROBLEM: EXTEND m^* DERIVATION TO 3-d.
(i.e., EFFECTIVE MASS)

HOW TO MEASURE m^*.



WILL PRODUCE CIRCULAR OR ELIPTICAL ORBITS.

MAGNETIC FIELD IN Z DIRECTION

$$\left.\begin{aligned} F_Y &= qV_X B = m_Y^* \ddot{Y} \\ F_X &= -qV_Y B = m_X^* \ddot{X} \end{aligned}\right\} \text{TWO D.E.}$$

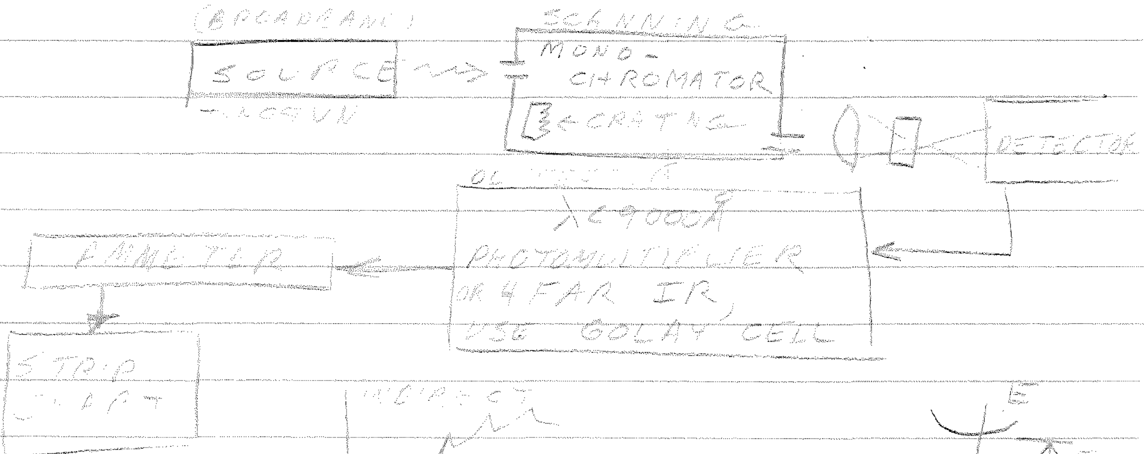
ASSUMING $m_X^* = m_Y^*$ (NOT ALWAYS TRUE):

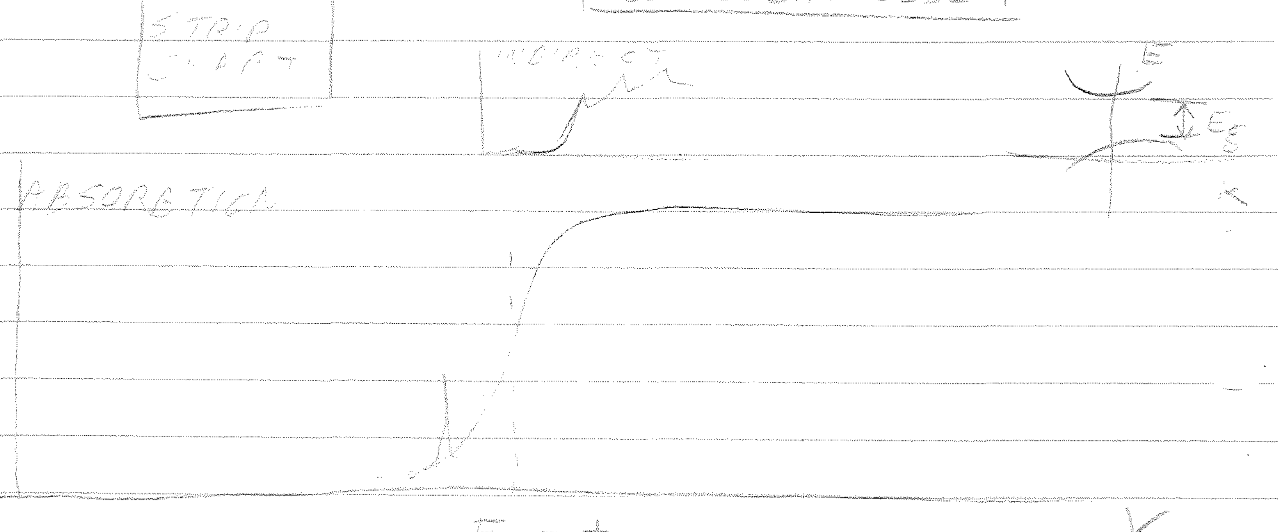
$$m(\ddot{X} + \ddot{Y}) = qB(\dot{X} - \dot{Y})$$

ASSUME $X = \sin \omega_0 t$, $Y = \cos \omega_0 t$

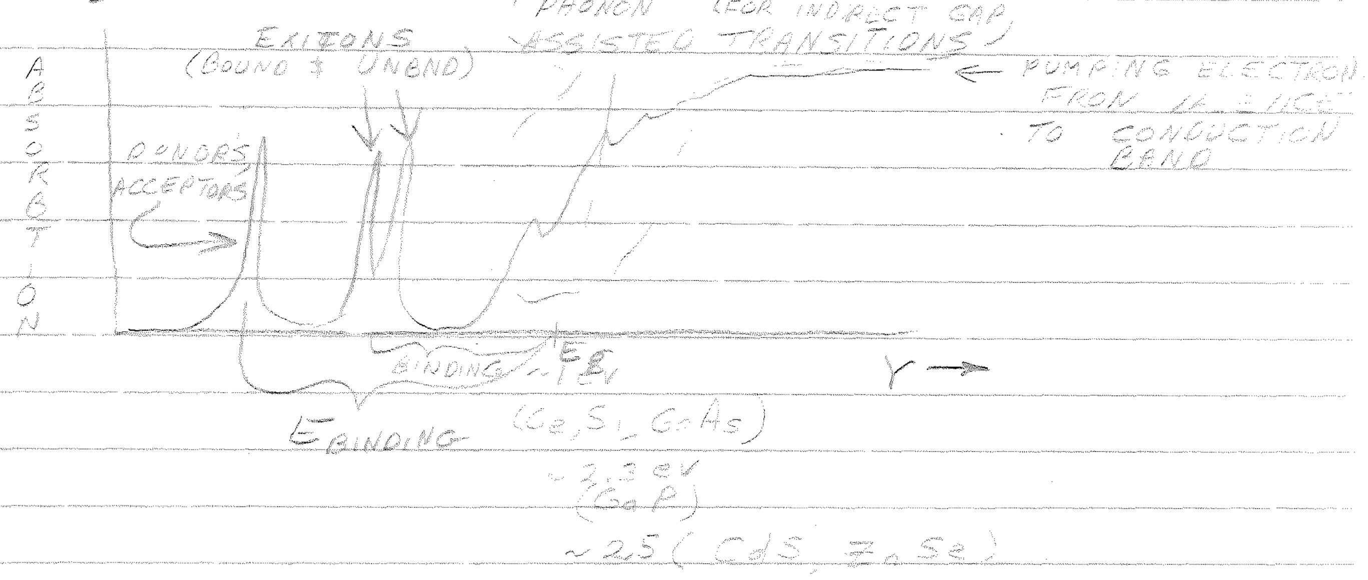
GIVES $\omega_0^2 = (qB/m^*)^2$

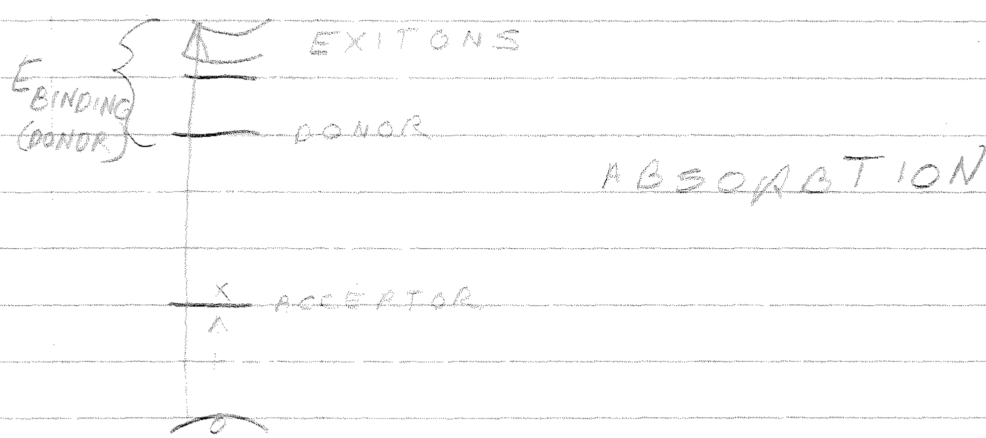
ABSORBTION MEASUREMENTS





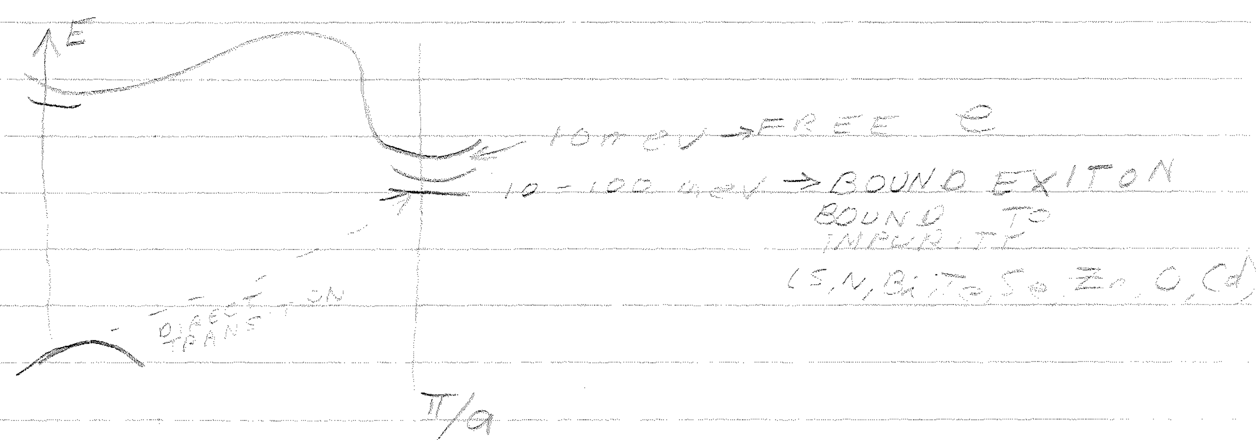
10-3-75 (FRI)

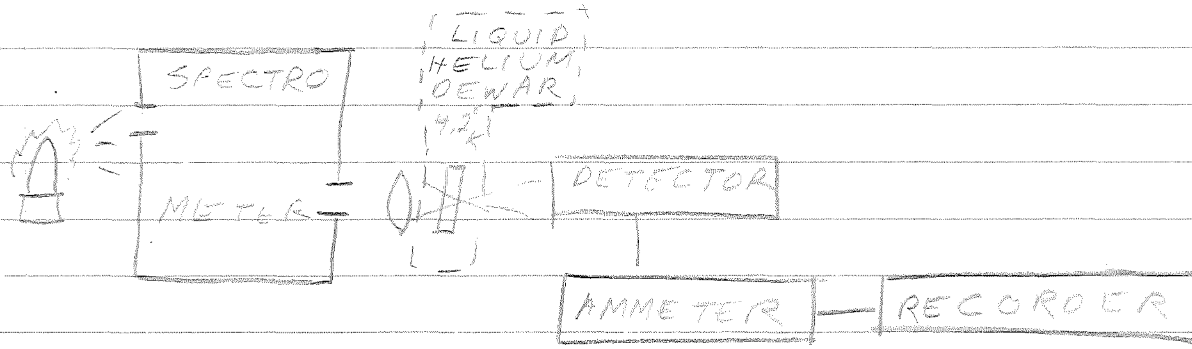




EXITON ~ e + h

EXITONS IN AN INDIRECT GAP MATERIAL

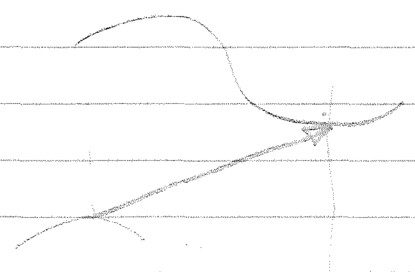




$1^\circ K \cong 1\,meV$

FOR USE:

NEP = NOISE EQUIVALENT PWR = $\int_E \frac{\delta}{\delta E}$ (FERMI-DIRAC DISTRIBUTION)

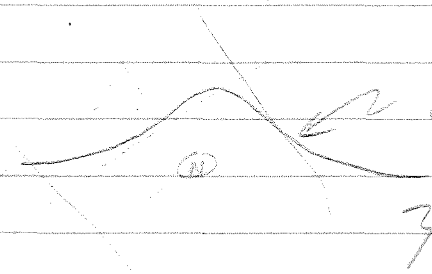


$h\nu \rightarrow e + h +$ PHONON

$$\frac{h\nu}{c} = \hbar\vec{k}_e + \hbar\vec{k}_h + \hbar\vec{k}_{phon.}$$

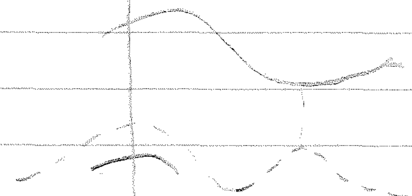
~ 0

GaP



EXITON WAVE FUNCTION: ψ

$$\psi(x) = \sum_k a_k e^{ikx}$$



IN K SPACE

$$\int \psi_f^* V(r) \psi_i = \int e^{-ik_f x} (\ ) e^{ik_i x}$$

$$\int e^{i(\vec{k}_i - \vec{k}_f)\cdot x} dx = \delta(k_i - k_f)$$

$\Rightarrow$ FINAL AND INITIAL K MUST BE EQUAL (CONS. OF MOMENTUM)

USE FOURIER ANALYSIS LIBERLY.
MAKING MEASUREMENTS (ABSORBTION)
CAN GIVE BINDING ENERGY

FERMI-DIRAC DISTRIBUTION

n = # ELECTRONS IN CONDUCTION BAND
p = # HOLES IN VALENCE BAND

$n = P_{FD}\,\varrho(E) \Rightarrow P_{FD}$ = FERMI-DIRAC DISTRIBUTION
= P[ELECTRON HAS ENERGY E
(W/O CONSIDERING SYSTEMS QUANTUM STATES]

$\varrho(E)$ = NUMBER OF QUANTUM STATES AS A FUNCTION OF ENERGY

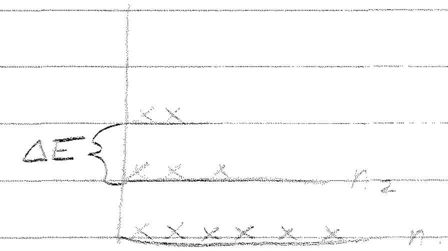
$n = \int n(E)\,dE = \int P\varrho\,dE$

P_{FD}

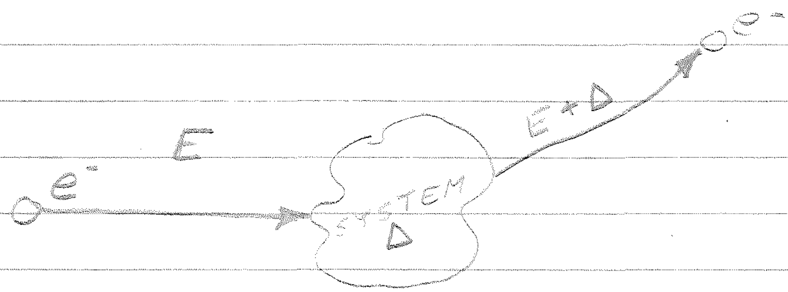
1) ASSUME THERMAL EQUALIBRIUM
2) ELECTRON PROPERTY (PAULI EXCLUSION PRINCIPLE) NOT MORE THAN ONE ELECTRON CAN HAVE A GIVEN SET OF QUANTUM #
$(E, l, S = \pm\frac{1}{2}, \text{ETC.})$ ANG. MOM $= \pm\frac{\hbar}{2}$

10-6-75 (MON)

FERMI - DIRAC DISTRIBUTION

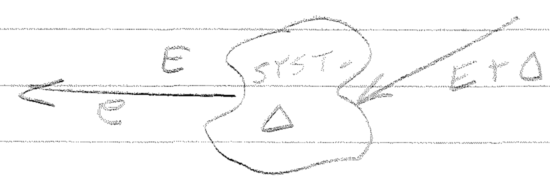


$$\frac{n_2}{n_1} \propto e^{-\frac{\Delta E}{kT}} = \text{BOLTZMAN FACTOR}$$



$P[e^- \text{ HAS ENERGY } E] \times P[E^- \text{ GOES TO } E+\Delta]$
$= f(E)\, P[E \to E+\Delta]$

$$\underbrace{f(E)\, p[E \to E+\Delta]}_{\text{CONSIDER REVERSE}} \underbrace{[1 - f(E+\Delta)]}_{\text{FROM PAULI ECLUSION}}$$



$\Rightarrow f(E+\Delta)$

$$\Rightarrow f(E)\, p[E \to E+\Delta][1 - f(E+\Delta)] = f(E+\Delta)\, P[E+\Delta \to E][1 - f(E)]$$

$$\frac{P[E \to E+\Delta]}{P[E+\Delta \to E]} = \frac{f(E+\Delta)\,[1 - f(E)]}{f(E)\,[1 - f(E+\Delta)]}$$

$$= e^{-\Delta E/kT}$$

SOLVE FOR $f(E)$

WHAT IS $f(E)$ = FERMI-DIRAC DIST. FUNC.

$$f(\xi) = \frac{1}{e^{\frac{E-E_c}{KT}} - 1}$$

① WHAT IS $n(E)$?
② WHAT IS n?

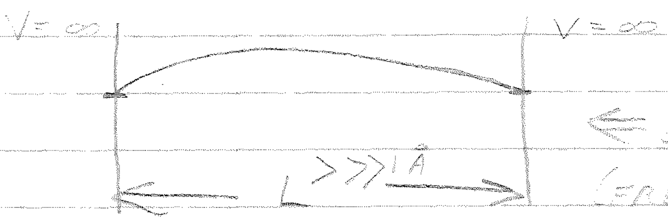
$n(E)$ = # ELECTRONS WITH ENERGY E
= $P[e^-$ CAN HAVE EN. E$]\, d\eta$ ← # BOXES TO PUT e^-'s IN
= $f(E)\, d\eta$

$$n = \int_{E_{BAND}} n(E)$$

DENSITY OF DONOR STATES = N_D^+ = DENSITY OF DONOR IONS

$$N_D^+ = N_D\left[1 - f(E_D)\right]$$

IN CONDUCTION BAND, e^- ACTS FREE.
DENSITY OF STATES FOR A FREE PARTICLE.



⟸ ONE DIMENSION (FREE PARTICLE IN A BOX)

LOWEST E ⟹ LONGEST λ

n	1	2	3	... n
λ	$2L$	L	$\frac{2}{3}L$	... $\frac{2L}{n}$
$K=\frac{2\pi}{\lambda}$ $(P=\hbar K)$	π/L	$\frac{2\pi}{L}$	$\frac{3\pi}{L}$	$\frac{n\pi}{L}$
$E=\frac{\hbar^2K^2}{2m}$	$\frac{\hbar^2\pi^2}{2mL^2}$	$\frac{2^2\hbar^2\pi^2}{2mL^2}$	$\frac{3^2\hbar^2\pi^2}{2mL^2}$	$\frac{n^2\hbar^2\pi^2}{2mL^2}$

$dn^{(1)}$ = # OF STATES 'TWIXT n & $n+m = m$

$$E_n = n^2\left(\frac{\hbar^2\pi^2}{2mL^2}\right)$$

$$n = \sqrt{\frac{2mEL^2}{\hbar^2\pi^2}} \Rightarrow dn = \frac{1}{2}\left(\frac{2mL^2}{\hbar^2\pi^2}\right)^{1/2}\frac{dE}{\sqrt{E}}$$

IN 3d WE GET

$$\frac{1}{8}(4\pi n^2 dn) = dn^{(3)}$$

GETS FIRST OCTANT OF A SPHERE SINCE $n > 0$

$$dn^{(3)} = 2\left(\frac{2mL^2}{\hbar^2\pi^2}\right)E\,\frac{\pi}{2}\,\frac{1}{2}\left(\frac{2mL^2}{\hbar^2\pi^2}\right)^{1/2}\frac{dE}{\sqrt{E}}$$

STUCK IN TO ALLOW FOR 2 SPIN STATES / ENERGY STATE

$$= \left(\qquad\right)\sqrt{E}\,dE$$

HOMEWORK: SOLVE FOR DENSITY IN TWO DIMENSIONS.
(FREE PARTICLE IN A L×L BOX)

NOW

$$n(E)\,dE = \frac{\pi}{2}\left(\frac{2m}{\hbar^2\pi^2}\right)^{3/2}\sqrt{E}\;\frac{1}{e^{\frac{E-E_f}{kT}}+1}\;dE$$

10-8-75 (WED)

$$n(E)\,dE = \text{CONST.}\ \frac{\sqrt{E}\ dE}{1 + e^{E-E_F/KT}}$$

FIND

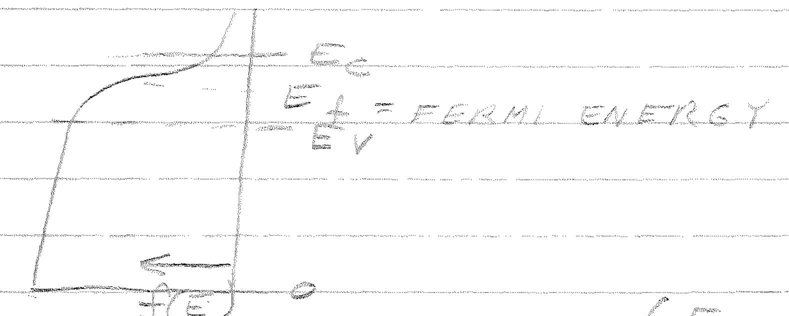
$$n = \int_{E_c}^{\text{TOP OF CONDUCTION BAND}} n(E)\,dE$$

$$= \text{CONS} \int_{E_c}^{\infty} \frac{\sqrt{E-E_c}}{1+e^{E-E_F/KT}}$$

$E_c - E_F \sim .2$ TO 1 eV

KT AT ROOM TEMP. ~ 0.026 eV

$$\Rightarrow n = \text{CONT} \int_{E_c}^{\infty} \sqrt{E-E_c}\ e^{-(E-E_F)/KT}\,dE$$



$$n = 2\left(\frac{2\pi m_e KT}{h^2}\right) e^{-\frac{(E_c - E_F)}{KT}}$$

$$= N_c\, e^{-(E_c - E_F)/KT}$$

= EFFECTIVE DENSITY OF STATES

p = # HOLES IN THE VALENCE BAND

$$= 2\left(\frac{2\pi m_h KT}{h^2}\right) e^{-(E_F - E_V)/KT}$$

$$= N_V\, e^{-(E_F - E_V)/KT}$$

MASS ACTION LAW

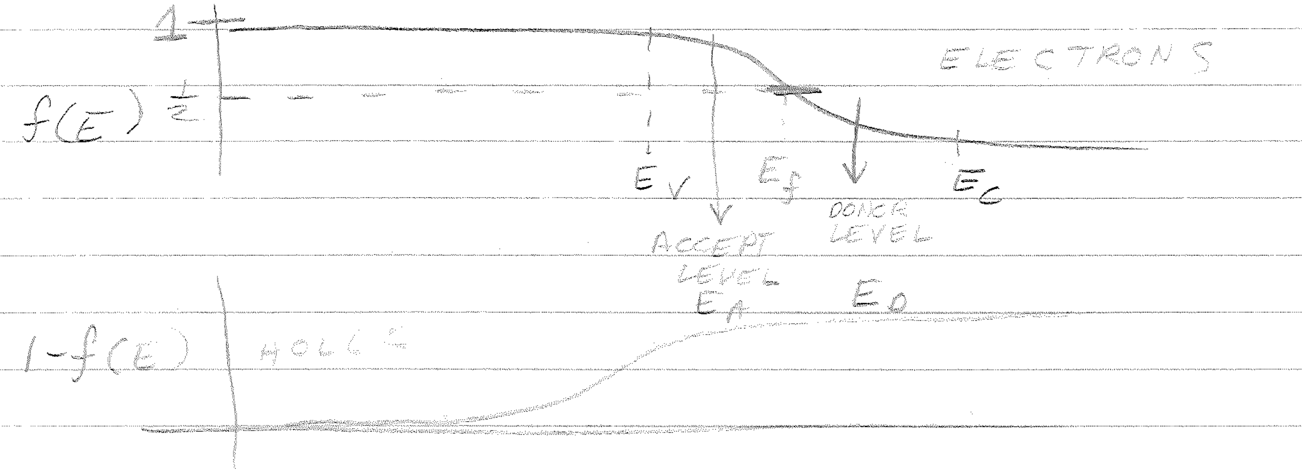
$$np = N_c N_V\, e^{(-E_F + E_V - E_c + E_F)/KT}$$

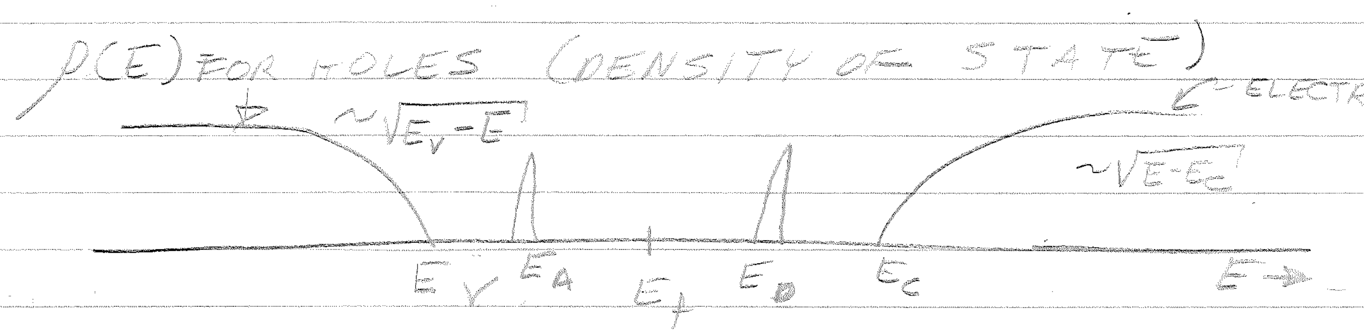
$$= N_c N_V\, e^{-E_g/KT}$$

E_g = ENERGY GAP = $E_c - E_V$

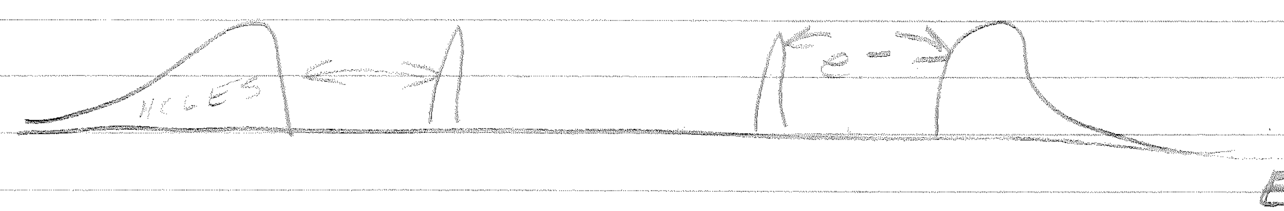
$$np = n_i^2$$

SUMMATION





$n(E) = (1 - f(E))\,\rho(E)$ FOR HOLES
$n(E) = f(E)\,\rho(E)$ FOR ELEC



HOMEWORK: FIND SOME STUFF
YOU CAN CALCULATE
WITH REAL NUMBERS.
"RELATE RESULTS TO REAL
NUMBERS. WHAT KIND OF
THINGS CAN YOU CALCULATE"

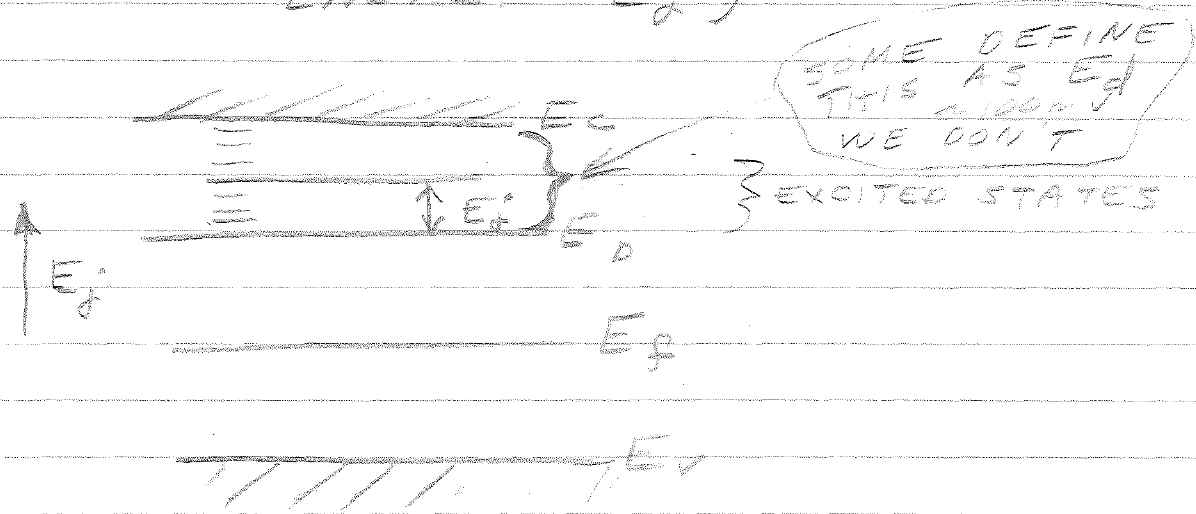
10-10-75 (FRI)

IMPURITY DISTRIBUTION FUNCTION
(DONORS – ACCEPTORS FOR HOMEWORK)

$f_j \triangleq P$[ELECTRON IS IN STATE j (OF THE DONOR SEMICONDUCTOR COMPLEX)]

ASSUME 1 ELECTRON (e^-) ON DONOR.

$f_j = P$[NO ELECTRON IS ALREADY BOUND TO THE DONOR]
$\times P$[AN ELECTRON HAS ENERGY E_j]



$$f_j = \left[1 + \sum_{i \neq j} f_i\right] \left\{ \frac{1}{1 + e^{(E_D + E_j - E_F)/kT}} \right\}$$

DEFINE $(E_D + E_j - E_F)/kT = \mathcal{J}$

FOR AN ACCEPTOR:
$(E_F - E_A - E_j)/kT = \mathcal{J}_a$

$$f_j = \left[1 + f_j - \sum_i f_i\right]\left(\frac{1}{1+e^{\mathcal{J}}}\right)$$

$$f_j\left[1 - \frac{1}{1+e^{\mathcal{J}}}\right] = \left[1 - \sum_i f_i\right]\left(\frac{1}{1+e^{\mathcal{J}}}\right)$$

$$= f_j\left(\frac{e^{\mathcal{J}}}{1+e^{\mathcal{J}}}\right) = F^+\left(\frac{1}{1+e^{\mathcal{J}}}\right)$$

WHERE $F^+ = P$[DONAR ATOM HAS NO ELECTRON (i.e. IS IONIZED)]

$$f_i = F^+ e^{-\mathcal{J}}$$

$F^+ + F^0 = 1$ ⇐ REQUIREMENT

WHERE $F^0 = P$[DONAR HAS AN ELECTRON]

$$= \sum_i f_i$$

$$F_0 = F^+ \sum_{\mathcal{J}} e^{-\mathcal{J}}$$

$$= (1 - F^+)$$

GIVES $F^+(1 + \sum e^{-\mathcal{J}}) = 1$

$$F^+ = \frac{1}{1+\sum e^{-\mathcal{J}}} = \frac{n_D}{N_D}$$

n_D = # e^- IN CONDUCTION BAND FROM DONORS

N_D = CONCENTRATION OF DONOR ATOMS.

TO INCLUDE DEJENERACY

LET g_j = # OF STATES WITH ENERGY E_j

$$F^{+} = \frac{1}{1+\sum_{\text{ENERGY } j} g_j e^{-\ell}}$$

$$F^{+} \simeq \left[1 + g_{grd} e^{-\ell_{grd}}\right]^{-1}$$

THUS

$$F^{0} = 1 - F^{+}$$

$$= \frac{g_{grd} e^{-\ell_{grd}}}{1 + g_{grd} e^{-\ell_{grd}}}$$

$$= \frac{1}{1 + \frac{1}{g_{grd}} e^{\ell_{grd}}}$$

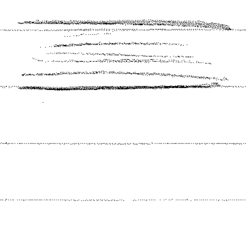
FOR ONE STATE

$$F^{0} = \frac{1}{1 + \frac{1}{g} e^{(E_D - E_F)/kT}}$$

AND

$$F^{+} = \frac{1}{1 + g e^{(E_F - E_D)/kT}}$$

ON TOP OF PAGE WE APPROX: $F^{+} \simeq \frac{1}{1 + g_j e^{\ell}}$



E_C

$$F^{+} = \frac{1}{1 + g_{GRD} e^{-\ell_{GRD}} + g_1 e^{-\ell_1} + \dots}$$

$$\ell_{GRD} = E_D - E_F$$

$$\ell_1 = E_D - E_F + E_1$$

$$\vdots \qquad \vdots$$

NEGLECT THE HIGHER ORDER TERMS WHICH ARE SMALL.

PROBLEM: DERIVE FOR ACCEPTORS

EFFECTS OF DOPING ON FERMI ENERGY

n = # OF ELECTRONS IN CONDUCTION BAND

$$= N_c e^{-(E_c - E_F)/kT}$$

NEUTRALITY DICTATES

$N_D - N_D^0$ = # DONORS IONIZED

$$n = (N_D - N_D^0) + p \qquad n >> p$$

p = ACCEPTOR CONCENTRATION

$$\Longrightarrow n \simeq N_D - N_D^0$$

$$N_c e^{-\frac{(E_c - E_F)}{kT}} = N_D\left[1 - \frac{1}{1 + \frac{1}{g} e^{(E_D - E_F)/kT}}\right]$$

$$= N_D \frac{1}{1 + g e^{(E_f - E_D)/kT}}$$

NORMALLY SOLVE FOR E_f. CONSIDER SOME CASES

1. HIGH TEMP

$$\Rightarrow \frac{N_D g}{N_c e^{-(E_c - E_D)/kT}} << 1$$

$$\Rightarrow E_f \simeq E_c - kT \ln \frac{N_c}{N_D}$$

2. LOW TEMP.

$$\frac{N_D g}{N_c e^{-(E_c - E_D)/kT}} >> 1$$

$$E_f \simeq \frac{E_c - E_D}{2} + \frac{kT}{2} \ln\left(\frac{N_c g}{N_D}\right)$$

GENERAL EXPRESSION FOR FERMI ENER.

$$N_c e^{-\frac{(E_c - E_F)}{kT}} = \frac{N_D}{1 + \sum g_i e^{(E_f - E_D - E_i)/kT}} + N_v e^{\frac{-(E_F - E_v)}{kT}}$$

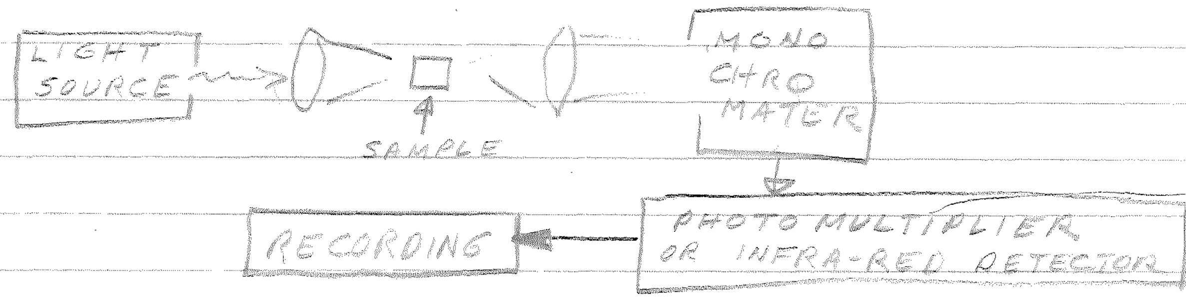
END OF MATERIAL COVERED ON TEST 1.

10-13-75 (MON)

SEMINAR @ 3:30 TODAY
ON RESONANCE RAMAN EFFECT.

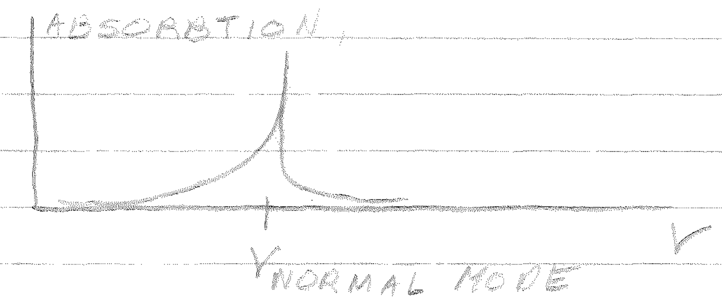
RAMAN EFFECT

INFRARED ABSORPTION / RAMAN EFFECT



CONSIDER HCl

H^+ —— Cl^- $\sim f \sim 3500\ cm^{-1}$
LIGHT (ν)
GENERATES DIPOLE MOMENT



$\vec{P} = \overleftrightarrow{\alpha} \cdot \vec{E} \Rightarrow \overleftrightarrow{\alpha}$ = TENSOR DIPOLE MOMENT

$$\alpha_{xy} = \alpha_{xy_0} + \sum_i \alpha_{xy_i} U_i + \sum_{ij} \alpha_{xy_{ij}} V_i V_j + \dots$$

U_j = NORMAL MODE =
$= U_{j0} \cos(\omega_j t + \beta_i)$

$\vec{P}$ = INDUCED POLARIZATION, E = APPLIED E FIELD

SUPPOSE $E = E_0 \cos \omega t$ (VISIBLE) $\omega \gg \omega_j$

$$P = \left[\alpha_{xy} + \sum \alpha_{xy_j} V_{j0} \cos(\omega_j t + \beta_j)\right] \times E_0 \cos \omega t$$

GETS

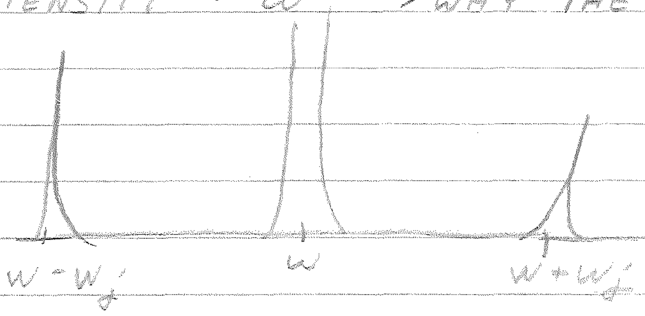
$$P = \alpha_{xy_0} E_0 \cos \omega t + \frac{E_0}{2} \sum_j \alpha_{xy_j} V_{j0} \times \left[\cos\{(\omega+\omega_j)t + \beta_j\} + \cos\{(\omega-\omega_j)t - \beta_j\}\right]$$

FIRST ORDER: $P^{(1)}(\omega) \sim \cos\omega t$ IF $\alpha_{xyo} \neq 0$

SECOND ORDER: $P^{(2)}(\omega \pm \omega_j) \equiv \cos[(\omega \pm \omega_j)t]$

IF $\alpha_{xyj} \neq 0$

I = INTENSITY $\sim \omega^4$ → WHY THE SKY IS BLUE!



$$\hbar\omega_{IN} - \hbar\omega_j = \hbar\omega_{OUT}$$

WHEN DOES RAMAN SCATTERING OCCUR?

$$P(\omega - \omega_j) = d\, E(\omega)\, E(\omega_j)$$

↑ FROM INTRINSIC MATERIAL PROPERTIES

$$-P = d'\,(-E(\omega))(-E(\omega_j))$$

IF THE CRYSTAL (GAS) HAS INVERSION SYMMETRY, THEN

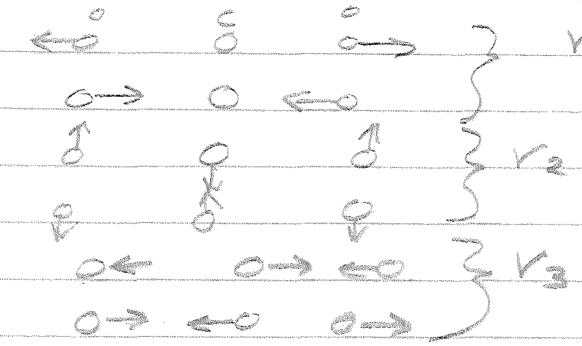
$d = d'$, THEN $d = 0$ AND

$$P(\omega - \omega_j) = -P(\omega - \omega_j)$$

ie $\alpha_{xyj} = 0$

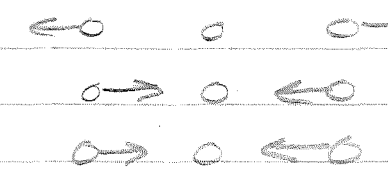
APPLICATION TO CO_2

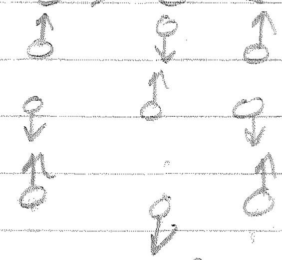
WHICH NORMAL MODES OF CO_2 ARE RAMAN ACTIVE

MODES: 

1) CHANGE PHASE BY 180°
AND REFLECT THROUGH OF C N

2) FOR RAMAN SCATTERING,
MOLECULE MUST BE DIFFERENT
FOR $d \neq 0$ (RAMAN ACTIVE)

ν_1: 
180°
REFECT $\Rightarrow$ RAMAN ACTIVE

ν_2: 
180°
REFLECT $\Rightarrow$ NOT RAMAN ACTIVE

ν_3: NOT RAMAN ACTIVE

FOR MORE COMPLICATED ATOMS, MUST
USE GROUP THEORY

10-15-75 (WED)

TEST: TEST ON WEDNESDAY, 10-22-75
MATERIAL UP TO LAST FRIDAY
CLOSED BOOK

HEAT CAPACITY:

DEF: HEAT CAPACITY $\equiv C_V = \left.\frac{\delta E}{\delta T}\right|_V$

IN A GAS

$$E \simeq 3NkT \Rightarrow C_V = 3Nk$$

PHONON AND ELECTRON CONTRIBUTION WILL BE LOOKED AT.

WHAT IS $\langle n_p(E)\rangle$ = AVE. # OF OSCILLATORS WITH ENERGY E

E = FOR A HARMONIC OSCILLATOR = $(n+\frac{1}{2})\hbar\omega$

USE BOLTZMAN FACTOR:

$$\frac{N_{n+1}}{N_n} = e^{-(E_{n+1}-E_n)/kT}$$

FOR HAR OSC: $\frac{N_{n+1}}{N_n} = e^{-\hbar\omega/kT}$

FRACTION OF FILLED STATES AT ENERGY $E_n = N_n \Big/ \sum_s N_s$

$$= \frac{e^{-E_n/kT}}{\sum_s e^{-E_s/kT}}$$

AVERAGE NUMBER OF QUANTA IN A STATE $n = \langle n\rangle$

$$\langle n\rangle = \frac{\sum_{n=0}^{\infty} n e^{-n\hbar\omega/kT}}{\sum_{n=0}^{\infty} e^{-n\hbar\omega/kT}}$$

LET $\hbar\omega/KT = X$

$$\Rightarrow \langle n \rangle = \frac{\sum_{n=1}^{\infty} n e^{-nx}}{\sum_{n=1}^{\infty} e^{-nx}}$$

NOTE: $n e^{-nx} = -\frac{d}{dx} e^{-nx}$

$$\frac{\sum_{n=1}^{\infty} n e^{-nx}}{\sum_{n=1}^{\infty} e^{-nx}} = \ln \sum_{n=0}^{\infty} e^{-nx}$$

LET $Y = e^{x} \Rightarrow \sum_{n=0}^{\infty} Y^n = S$

$$YS - S = 1$$

$$\Rightarrow S = \frac{1}{1-Y}$$

$$= \frac{1}{1-e^{x}}$$

$$= \frac{1}{1-e^{-\hbar\omega/KT}}$$

$$\frac{\delta}{\delta x}\left[\frac{1}{1-e^{-\hbar\omega/KT}}\right]$$

$$\langle n \rangle = \frac{1}{1-e^{-\hbar\omega/KT}}$$

$$= \frac{1}{e^{\hbar\omega/KT}-1} \Longleftarrow \text{OCCUPATION \# FOR } n^{TH} \text{ LEVEL}$$

$$= \frac{1}{e^{E/KT}-1} \Leftarrow \text{FOR BOSONS}$$

RECALL FERMI-DIRAC DISTRIBUTION:

$$\frac{1}{e^{E-E_F/KT}+1} \Leftarrow \text{FOR FERMIONS}$$
(INCLUDES PAULI EXCLUSION PRINCIPLE)

FOR SMALL $\hbar\omega$

$$\langle n \rangle \simeq \frac{1}{\left(1+\frac{\hbar\omega}{KT}\right)-1} = \frac{KT}{\hbar\omega}$$

THEN

$$\langle E \rangle = \langle n \rangle \hbar\omega = kT \Leftarrow \text{CLASSICAL RESULT}$$

GENERALLY

$$\langle E(\omega)\rangle = \frac{N\hbar\omega}{e^{\frac{\hbar\omega}{KT}} - 1}$$

THEN

$$C_v = \frac{\delta\langle E\rangle}{\delta T}\bigg|_v = Nk\left(\frac{\hbar\omega}{KT}\right)^2 \frac{e^{\hbar\omega/KT}}{(e^{\hbar\omega/KT}-1)^2}$$

IN 3D, WE GOT THREE DEGREES OF FREEDOM $\Rightarrow$ MULTIPLY C_v BY 3

[HOMEWORK: WHAT IS C_v FOR LARGE TEMPERATURE?]

$$E_{TOTAL} = \sum \hbar\omega\langle n\rangle$$
$$= \int \hbar\omega\langle n\rangle\left(\frac{dn}{dE}\right)dE$$

DEBYE USED DENSITY OF STATES

$$\frac{dn}{dE} = \frac{(\text{Volume})\,\omega^2}{2\pi^2\hbar V^3} \quad ; V = \text{VELOCITY}$$

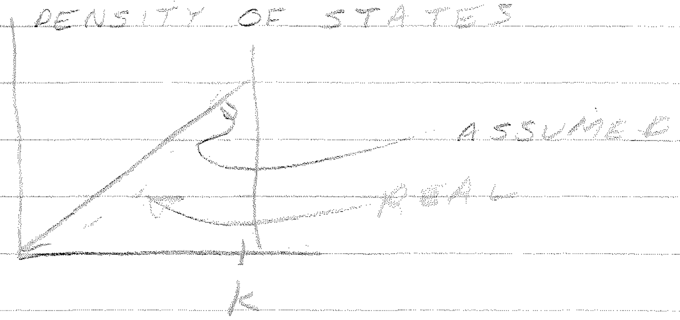
$\omega = VK \Leftarrow$ ASSUMPTION OF DISPERSION RELATION

ω_D = DEBYE FREQUENCY = MAXIMUM ALLOWABLE FREQ.

$$3N = V\omega_D^{2}/2\pi^2\hbar V^3$$

$$\Rightarrow \omega_D = \frac{6\pi^2 V^3 N}{(\text{VOL})}$$

DENSITY OF STATES



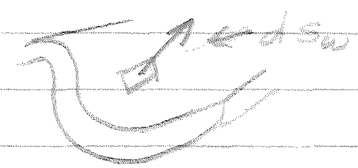
10-17-75 (FRI)

$$C_V = \frac{\delta}{\delta T}\langle E\rangle\Big|_V = Nk\left(\frac{\hbar\omega}{kT}\right)^2 \frac{e^{\hbar\omega/kT}}{(e^{\hbar\omega/kT}-1)^2}$$

$$E = \int_0^{\omega_0} \hbar\omega\, \mathcal{D}(\omega)\, n(\omega)\, d\omega$$

ΔK = KIND OF DENSITY OF STATES IN A BOX $= \frac{2\pi}{L}$ (ONE DIMENSION)

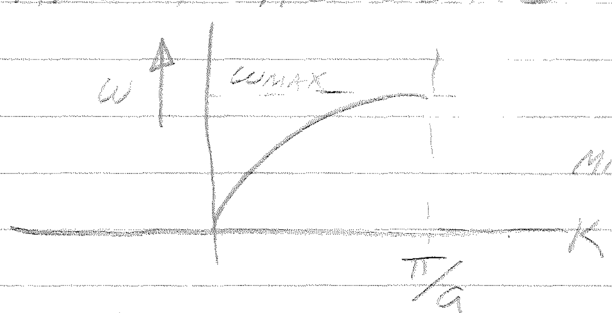
GIVES $\mathcal{D}(\omega)d\omega = \frac{L}{\pi}\frac{dK}{d\omega}d\omega$



GIVES ; $D(\omega) = \frac{V}{(2\pi)^3}\int \frac{dS_\omega}{d\omega/dK}$

$\frac{d\omega}{dK}$ = WAVE PACKET GROUP VELOCITY

EXAMPLE: ACOUSTIC PHONON



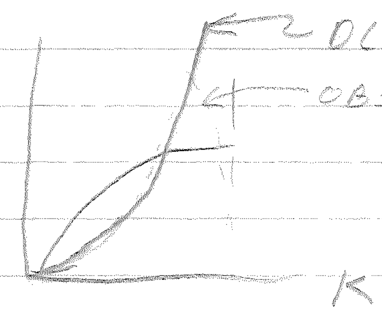
$\omega = \omega_{max} \sin\left(\frac{Ka}{2}\right)$

MAY FIND $D(\omega)$

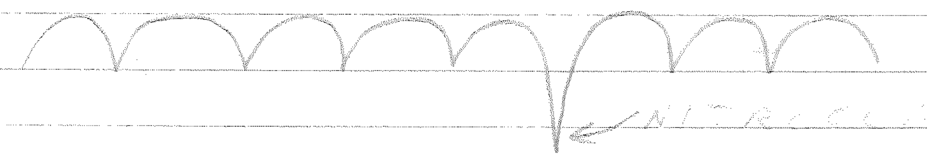
ONE CAN SHOW (EXTRA CREDIT HOMEWORK)

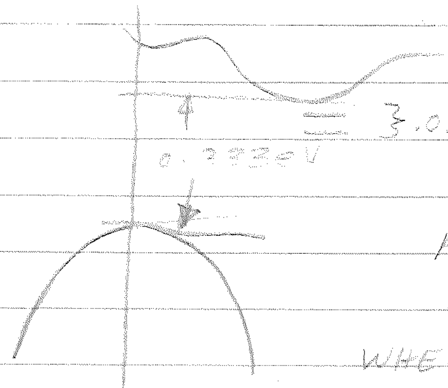
$$D(\omega) = \frac{2L}{\pi a}\left(\frac{1}{\omega_{max}^2 - \omega^2}\right)^{1/2}$$

MODEL BREAKS DOWN @ ω_{max}

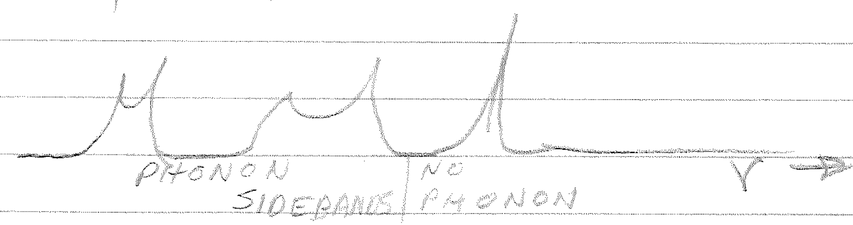


GaP:N GALLIUM PHOSPHIDE





AT 5°K, STRONG FLOURESCENCE WHEN e^- IS IN CONDUCTION BAND



BACK TO C_V.

RECALL: $E = \int_0^{\omega_D} d\omega \, \frac{V\omega^2}{2\pi^2 v^3}\left(\frac{\hbar\omega}{e^{\hbar\omega/kT}-1}\right)$

DEBYE ASSUMED THAT: $\omega = vk$ (i.e. ACOUSTIC PHONONS).

GIVES: $\omega_D^3 = 6\pi^2 v^3 N/\text{VOLUME}$

= DEBYE APPROXIMATION

$$E = \frac{3VK^4T^4}{2\pi^2 v^3 \hbar^3}\int_0^{x_D} x^3dx/(e^x-1) \Rightarrow x_D = \frac{\hbar\omega_D}{kT}$$

$x_D = \Theta_D/T$

Θ_D = DEBYE TEMPERATURE

THEN

$$C_V = 9NK\left(\frac{T}{\Theta_D}\right)^3\int_0^{x_D}\frac{x^4e^x\,dx}{(e^x-1)^2}$$

FOR SMALL T

$$E = \text{CONST} \times \int_0^{\infty}\frac{x^3dx}{e^x-1}$$

(CONT)

RECALL: $\frac{1}{e^{x}-1} = \sum_{n=1}^{\infty} e^{-nx}$

$\Rightarrow E = \text{CONST} \int_0^\infty dx\, x^3 \sum_{n=1}^{\infty} e^{-nx}$

INTEGRATING TERMWISE

$E = \text{CONST} \times 6 \sum_{1}^{\infty} \frac{1}{n^4}$

$= \text{CONST} \times \frac{6\pi^4}{15}$

THUS, FOR T SMALL

$C_V \triangleq \left.\frac{dE}{dT}\right|_V = \frac{12\pi^4}{5} NK \left(\frac{T}{\Theta_D}\right)^3$

SIGNIFICANT RESULT

ELECTRON CONTRIBUTION TO SPECIFIC HEAT

$E \sim \frac{3}{2} kTN \Rightarrow C_V \approx \frac{3}{2} k$

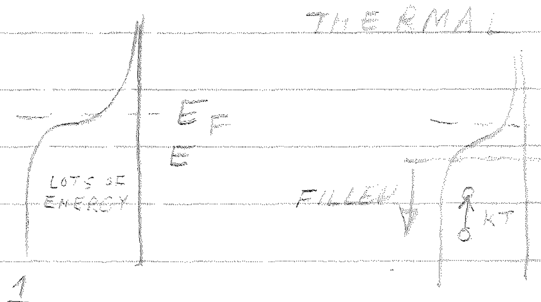
DIDN'T WORK OUT EXPERIMENTALLY

RECALL: $E_F = \frac{\hbar^2}{2m}(3\pi^2 n)^{2/3}$

$dN/dE = \frac{\text{VOL}}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\sqrt{E}$

THERMAL ENERGY $\sim kT$

$kT \sim \frac{1}{40}\, eV$



CAN'T DO THIS CAUSE OF PAULI EXCLUSION PRINCIPLE

% # OF AVAILABLE ROUGHLY: $\frac{T}{T_F} \sim 1\%$ FOR METAL

(THIS AGREED WITH EXPERIMENT)

10-20-75 (MON)

C_V ASSUMING FERMI-DIRAC:

$\Delta = \int_0^\infty E\, P_{FD}(E)\, dN/dE\, dE$

DENSITY OF STATES

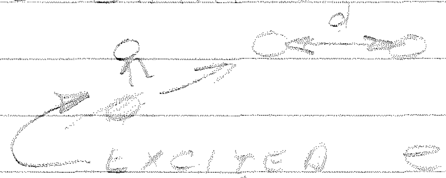
$- \int_0^{E_F} [\qquad] dE$ ← SUBTRACTS E BELOW E_F

THIS GIVES $C_V = \frac{d(\Delta E)}{dT} = \frac{\pi^2}{2} Nk\, T/T_F$

OFF AN ORDER OF ABOUT 5.

TEST QUESTIONS

e^- SHARING

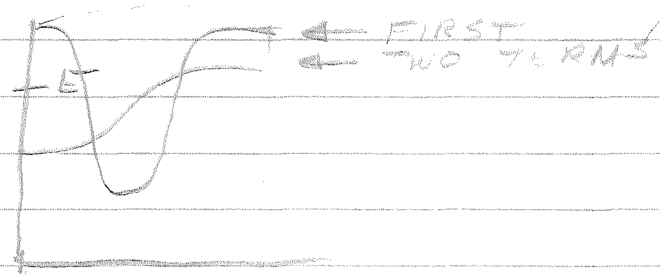


EXCITED e^- IN CONDUCTION BAND

$i\hbar \frac{\delta}{\delta t} a_0 = E a_0 + V_1 a_1 + V_2 a_2$
$+ V_1 a_{-1} + V_2 a_{-2} + \dots$

$V_1 a_1$ IS A FORM OF COUPLING.

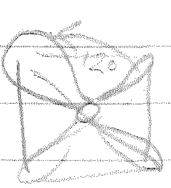
GIVES $E = E_0 \pm V_1 \cos kx_1 \pm 2V_2 \cos kx_2 + \dots$



V_1 AND V_2 ARE MEASUREABLE

FOR QUASI-FREE e^-: $E \sim \hbar^2 k^2/2m^*$

TETRAHEDRAN: 4 TRIANGLES



← Si, Ge, ...

SIMPLE HARMONIC OSCILLATOR

$V(x) = \frac{1}{2} m \omega^2 x^2 \quad ; \quad \omega = \sqrt{k/m}$

SCHRÖ'S EQN IS

$$-\frac{\hbar^2}{2m}\nabla^2\psi + \frac{1}{2}m\omega^2x^2\psi = E\psi$$

$$\frac{\delta^2\psi}{\delta x^2} + \frac{2m}{\hbar^2}\left(E - \frac{m\omega^2}{2}\right)\psi = 0$$

BRUTE FORCE SOLUTION.

LET $\sqrt{\frac{m\omega}{\hbar}}\, x = \xi$

$\mathcal{E} = {}^{2E}/\hbar\omega$

GIVES $\frac{d^2\psi}{\delta\xi^2} + (\mathcal{E} - \xi^2)\psi = 0$

THIS IS HERMITES DIFFERENTIAL EQN.

$$\psi = v(\xi)\, e^{-\xi^2/2}$$

GIVES

$$\frac{\delta^2 v}{\delta\xi^2} - 2\xi\frac{\delta v}{\delta\xi} + (\mathcal{E} - 1)v = 0$$

$$V(\xi) = \sum_{r=1}^{\infty} a_r \xi^r$$

PLUG ER IN

$$dv/\delta\xi = \sum_{1}^{\infty} r\, a_r\, \xi^{r-1} = \sum_{p=0}^{\infty} (p+1)\, a_{p+1}\, \xi^p$$

$$\delta^2 v/\delta\xi^2 = \sum_{2}^{\infty} r(r-1)\, a_r\, \xi^{r-2}$$

$$= \sum_{p=0}^{\infty} (p+2)(p+1)\, a_{p+2}\, \xi^p$$

$$\Rightarrow \sum_{r=0}^{\infty}\Big[(r+2)(r+1)\,a_{r+2} + \left[(\mathcal{E}-1) - 2r\right]a_r\Big]\xi^r = 0$$

$$\therefore (r+2)(r+1)\,a_{r+2} = \boxed{\left[2r - (\mathcal{E}-1)\right]a_r}$$

$$a_{r+2} = \frac{2r - (\mathcal{E}-1)}{(r+2)(r+1)}\, a_r$$

$\Rightarrow$ TWO INDEPENDENT SOLUTIONS

GOTTA KNOW a_0 AND a_1.

FIND BY NORMALIZATION.

TO KEEP THINGS (ψ) FROM BLOWING UP, WE MUST RESTRICT: $\mathcal{E} = 2n+1$

$$\frac{2E}{\hbar\omega} = \epsilon = 2n+1$$

$$\Rightarrow E = \hbar\omega\left(n+\frac{1}{2}\right) \Longleftarrow$$

10-24-75 (FRI)

TEST: STANDARD DEVIATION ~ 10

AVE ~ 67 TO 72

FERMI ENERGY: $E_F = \frac{E_G}{2} + (\ ) kT \ln(\ )$

NOTES: HARMONIC OSCILLATOR

$$V(x) = \frac{1}{2} m\omega^2 x^2$$

$$\psi = V(\xi) e^{-\xi^2/2} \qquad \xi = \sqrt{\frac{m\omega}{\hbar}}\, x$$

$$\Rightarrow E_n = \hbar\omega\left(n+\frac{1}{2}\right)$$

SOLUTION WAS HERMITE POLYNOMIALS

$$H = V(\xi) = \sum a_n \xi^n$$

$$a_{s+2} = \frac{2s+1-\epsilon_N}{(s+1)(s+2)} \qquad \epsilon_N = \text{NORMALIZED ENERGY}$$

$$H_0(\xi) = 1$$

$$H_1(\xi) = 2\xi$$

$$H_2(\xi) = 4\xi^2 - 2$$

$$H_3(\xi) = 8\xi^3 - 12\xi$$

ARE ORTHOGONAL: $\int_{-\infty}^{\infty} H_n(\xi) H_m(\xi)\, d\xi = 0$ FOR $m \neq n$

$$H_n(\xi) = (-1)^n e^{\xi^2} \frac{d^n\left(e^{-\xi^2}\right)}{d\xi^n}$$

GENERATING FUNCTIONS

RECURRSION:

$$\frac{dH_n(\xi)}{d\xi} = 2n H_{n-1}(\xi)$$

$$\psi_n = H_n e^{-\xi^2/2}$$

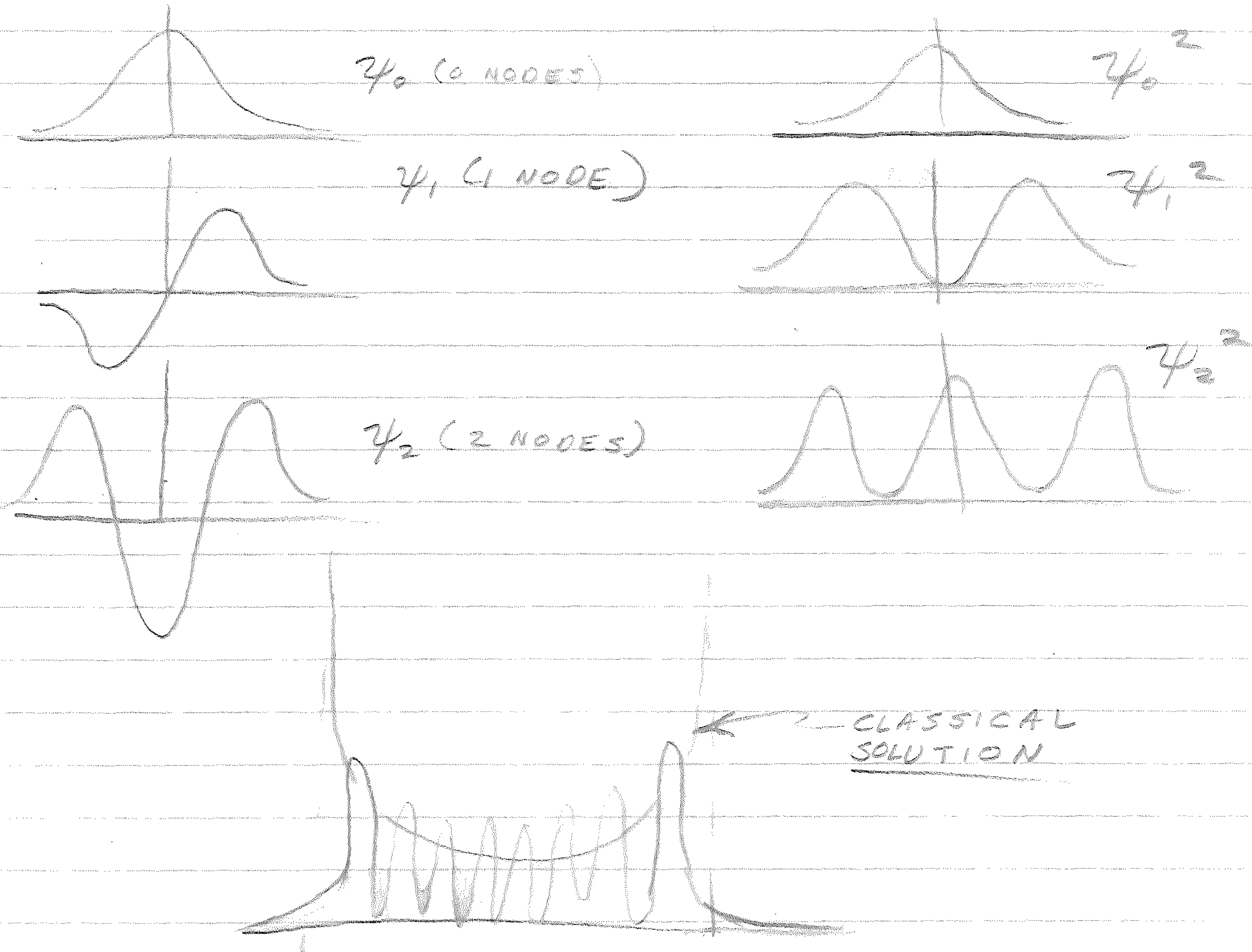
NORMALIZATION CONDITION:

$$\int_{-\infty}^{\infty} H_n^2(\xi)\, e^{-\xi^2}\, d\xi = \sqrt{\pi}\, 2^n\, n!$$

$$= 2n \int_{-\infty}^{\infty} H_{n-1}^2(\xi)\, e^{-\xi^2}\, d\xi$$

PROBLEM: SHOW THE ABOVE (DUE WEDNESDAY)

OSCILLATOR WAVE FUNCTIONS:



$$\sqrt{n+1}\, \psi_{n+1} - \sqrt{2}\, \xi \psi_n + \sqrt{n}\, \psi_{n-1} = 0$$

$$\xi \psi_n + \frac{d\psi_n}{\delta x} = \sqrt{2n}\, \psi_{n-1}$$

$$\xi \psi_n - \frac{\delta \psi_n}{\delta x} = \sqrt{2(n+1)}\, \psi_{n+1}$$

MATRIX ELEMENT

$\langle \psi_F | \text{PERT} | \psi_i \rangle$

$\psi_i = \phi_i(\text{ATOM})\, \Delta_i(\text{FIELD})$

DIPOLE: $V = e\bar{x}$

$\langle \psi_n' | e\bar{x} | \psi_i \rangle$

ADD RECURRANCE RELATION:

$2\xi \psi_n = \sqrt{2(n+1)}\, \psi_{n+1} + \sqrt{2n}\, \psi_{n-1}$

$\int \psi_{n+1} \xi \psi_n = \sqrt{2(n+1)}$

$\int \psi_{n-1} \xi \psi_n = \sqrt{2n}$

FERMI'S GOLDEN RULE
(RATE OF TRANSITION)

CROSS-SECTION: Θ

RECALL: $\psi(x,t) = \sum_n a_n \phi_n e^{-i\omega_n t}$

SOLUTION OF $H\psi = E\psi$

PERTURB: V

ASSUMED: $a = a(t)$

(?) $a_s(t) = -\frac{i}{\hbar} \sum' a_n \int V_{sn}(t) e^{-\frac{i}{\hbar}(E_s - E_n)t}\, dt$

ANYWAY, WE GET THE FOLLOWING RATE OF CHANGE

$$r(t) = \frac{2\pi}{\hbar} |V_{sn}|^2 \rho(E_n)$$

10-27-75 (MON)

FERMI'S GOLDEN RULE

$$\psi = \sum a_n(t)\phi_n(x)\, e^{-i/\hbar E_n t}$$

SOLUTION TO $H\psi = E\psi = \frac{i}{\hbar}\frac{\delta \psi}{\delta t}$

ASSUME $a = a(t)$

SOLVE THIS PERT. PROBLEM: $(H+V)\psi = E\psi$

GIVES EXACTLY:

$$\frac{\delta a_s}{\delta t} = -\frac{i}{\hbar}\sum_n a_n V_{sn}\, e^{\frac{i}{\hbar}(E_s - E_n)t}$$

$$V_{sn} = \int \phi_s^* V \phi_n \, d\vec{x}$$

ASSUME $\Delta a_s(t)$ ARE SMALL

THEN $a_n(t) \doteq a_n(0) = a_n$

ASSUMING SYSTEM IS INITIALLY IN STATE n:

$$a_n(0) = 1 \doteq a_n(t)$$

$$a_s(t) = -\frac{i}{\hbar}\int_0^t V_{sn}\, e^{\frac{i}{\hbar}(E_s - E_n)t}\, dt$$

ASSUMING V IS NOT A FUNCTION OF TIME

i.e. $V_{sn} \neq V_{sn}(t)$

THEN

$$a_s(t) = -V_{sn}\frac{e^{\frac{i}{\hbar}(E_s - E_n)t} - 1}{E_s - E_n}$$

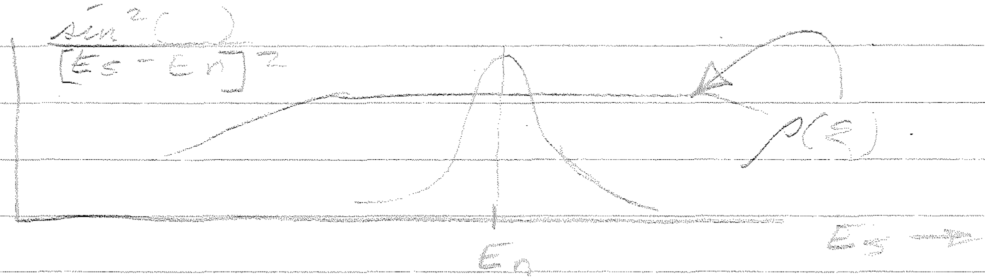
$$P[\text{BEING IN STATE } s] = P_s = |a_s(t)|^2$$

$$= 4|V_{sn}|^2 \frac{\sin^2\left[\frac{t}{2\hbar}(E_s - E_n)\right]}{(E_s - E_n)^2}$$

$$P(t) = \sum_s P_s(t)$$

$$\simeq \int_s 4|V_{sn}|^2 \frac{\sin^2\left[\frac{t}{2\hbar}(E_s - E_n)\right]}{(E_s - E_n)^2}$$

$$\rho(E_s - E_n)\, d(E_s - E_n)$$



SO, OVER REGION OF INTEREST

LET $\rho(E_s - E_n)$ = DENS OF STATE $\approx \rho(E_n)$

$$P(t) \cong 4|V_{sn}|^2 \rho(E_n) \int_{-\infty}^{\infty} \frac{\sin^2\left[(E_s - E_n)t/2\hbar\right]}{(E_s - E_n)^2} \times d(E_s - E_n)$$

[HOMEWORK: SOLVE INTEGRAL]

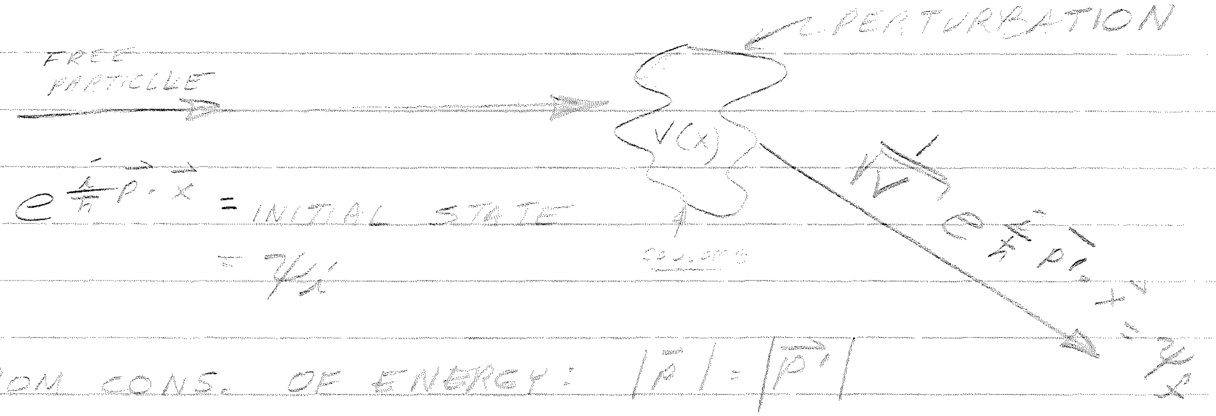
ANSWER IS

$$P(t) = \rho(E_n) \frac{2\pi}{\hbar} |V_{sn}|^2 t$$

AND RATE OF TRANSITION

$$\underline{\frac{dP(t)}{dt} = \frac{2\pi}{\hbar} |V_{sn}|^2 \rho(E_n)} \Longleftarrow \text{FERMI'S GOLDEN RULE \#2}$$

EXAMPLE: RUTHERFORD SCATTERING



$\frac{1}{\sqrt{Vol}} e^{\frac{i}{\hbar}\vec{p}\cdot\vec{x}}$ = INITIAL STATE $= \psi_i$

FROM CONS. OF ENERGY: $|\vec{p}| = |\vec{p}'|$

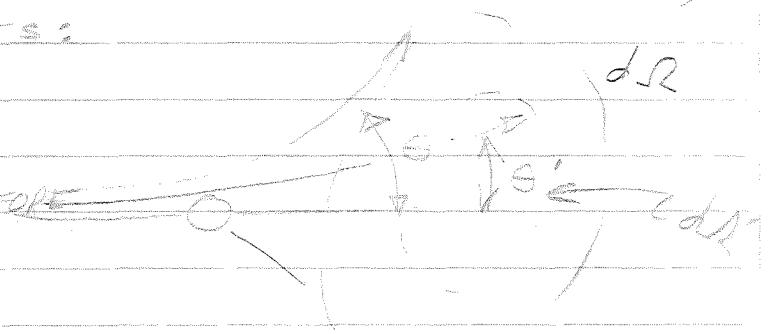
$$V_{sn} = \frac{1}{V}\int V(x)\, e^{\frac{i}{\hbar}(\vec{p}-\vec{p}')\cdot x}\, d^3x$$

$$= \frac{1}{V} \mathcal{F}[V(x)]$$ ⟸ FOURIER TRANSFORM

DENSITY OF STATES:

$$\frac{Vp^2\,dp\,d\Omega}{(2\pi\hbar)^3 dE}$$

($d\Omega$ INTEGRATED OUT BEFORE)



RATE OF TRANSITION = $\frac{d\Omega\, v}{Vol}\;\frac{d\sigma}{d\Omega}$

$d\Omega$ = CROSS SECTION

$d\sigma$ = % GOING INTO $d\Omega$

RATE OF TRANSITION = $\frac{2\pi}{\hbar}\left|\frac{1}{Vol} V(\mathcal{F}t)\right|^2$

$$\times \frac{Vp^2\,d\Omega}{8\pi^3\hbar^3 v}$$

GIVES $$\frac{d\sigma}{d\Omega} = \frac{1}{4\pi^2\hbar^4}\frac{p^2}{v^2}\left|V_{p,p'}\right|^2 \Longleftarrow$$

$\frac{p^2}{v^2} = m^2$ NON-RELATIVISTICALLY

FOR A COULOMB POTENTIAL:

$$V(r) = zZe^2/r \quad \text{(GAUSSIAN UNITS)}$$

$$V_{p-p'} = zZ \int \frac{1}{r} e^{\frac{i}{\hbar}(\vec{p}-\vec{p}')\cdot\vec{x}} \, d^3x$$

THIS IS SOLVED IN JACKSON (FIELDS TEXT)

GIVES

$$V_{p-p'} = \pi\hbar^2 zZe^2 / (4p^2 \sin^2 \theta/2)$$

WHICH IN TURN GIVES

$$\frac{d\sigma}{d\Omega} = \frac{z^2 Z^2}{4} \left(\frac{me^2}{p^2}\right)^2 \frac{1}{\sin^4 \theta/2}$$

SAME AS RUTHERFORD'S SOLUTION.

HEAT DIFFUSION EQUATION:

$$\nabla^2 T = \frac{\rho c}{K} \frac{\delta T}{\delta t}$$

K = THERMAL CONDUCTIVITY

ρ = DENSITY

C = HEAT CAPACITY

10-29-75 (WED)

(READ CHAPT. 3)

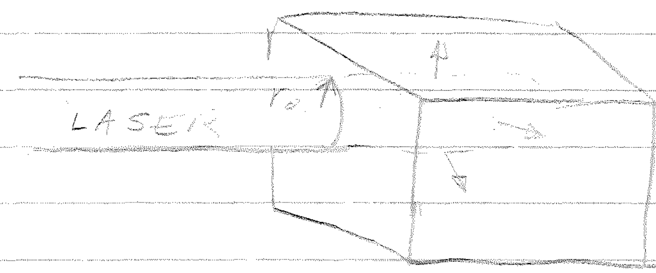
HEAT DIFFUSION EQUATION:

$$\nabla^2 T = \frac{\rho c}{K} \frac{\partial T}{\partial t}$$

ρ = DENSITY

C = SPECIFIC HEAT

K = THERMAL CONDUCTIVITY

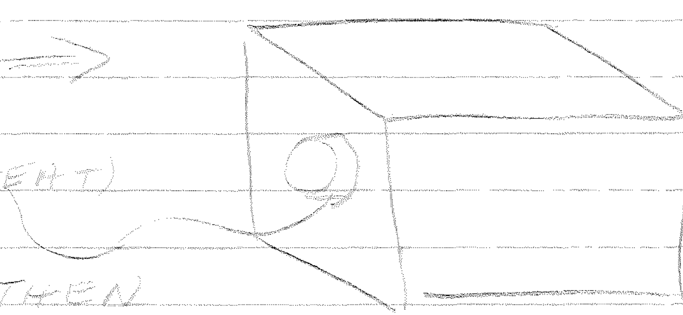


ASSUME BEAM IS GAUSSIAN:

$$I = I_0 e^{-\frac{r^2}{2 r_0^2}}$$

① RADIAL HEAT

② ABSORBTION ⟹



ENERGY (HEAT) ABSORBED AT SURFACE THEN TRANSMITTED

FOR CASE 1: (RADIAL)

USE CYLINDRICAL COORDINATES

$$\frac{\delta T}{\delta z} = 0, \quad \frac{\delta T}{\delta \theta} = 0$$

GIVES:

$$\frac{\rho c}{K} \frac{\delta T}{\delta t} = \frac{1}{r} \frac{\delta}{\delta r} \frac{r \, \delta T}{\delta r}$$

USE SEPERATION OF VARIABLES:

$$T(r,t) = T_r(r) \, T_t(t)$$

$$\frac{\rho c}{K} \frac{\delta T}{\delta t} = \frac{1}{r} \frac{\delta}{\delta r} r \frac{\delta T}{\delta r}$$

GIVES

$$\frac{1}{r} \frac{\delta}{\delta r} r \frac{\delta T_r}{\delta r} = -U^2 T_r \quad \text{(BESSEL'S EQ'N)}$$

$$\frac{\rho c}{K} \frac{\delta T_t}{\delta t} = -U^2 T_t$$

GIVES

$$T_r = A(U) \, J_0(rU)$$

$$T_t \propto e^{-U^2 K T / \rho c}$$

$$\therefore T = T_r T_t = A(U) \, J_0(rU) \, e^{-U^2 K T / \rho c}$$

APPLY BOUNDARY CONDITIONS:

$$T(r, t=0) = T_0 \, e^{-r^2 / 2 r_c^2}$$

GIVES (FOURIER BESSEL TRANSFORM)

$$e^{-r^2/2r_c^2} = \int_0^\infty A(U) \, J_0(Ur) \, dU$$

$$A(U) = \int_{-\infty}^{\infty} r \, dr \, e^{-\frac{r^2}{2r_c^2}} J_0(Ur)$$

$$T(r,t) = \int_0^\infty A(U) \, e^{-U^2 K T / \rho c} \, U J_0(Ur) \, dU$$

$$T(r,t) = \int_0^\infty u\,du \left\{ \int_0^\infty x\,dx\, J_0(ux)\, e^{-\frac{x^2}{2r_0^2}} dx \right\}$$

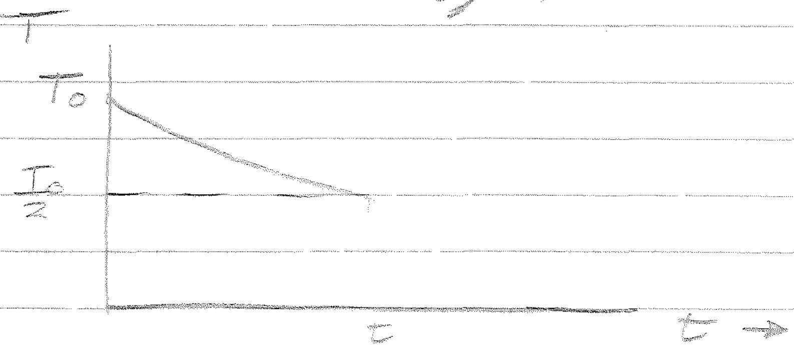
$$\times e^{-u^2 kt/\rho c}\, J_0(ur)\, dr$$

FOR SOLUTION, SEE WATSON (13.3) GIVES

$$T(r,t) = r_0^2 \int_0^\infty u\,du\, J_0(ur)\, e^{-\left(\frac{kt}{\rho c} + \frac{r_0^2}{2}\right)u^2}$$

$$= T_0 \frac{1}{\left(1 + \frac{2kT}{r_0^2 \rho c}\right)} \times e^{-\frac{\alpha r^2}{\rho r_0^2}}$$

$$\alpha = \left(1 + \frac{2kt}{\rho c r_0^2}\right)^{-1}$$



$$\frac{T(r,t)}{T(r,t=0)} = \frac{1}{2}$$

$r = 0$ GIVES $\frac{2kT}{r_0^2 \rho c} = 1$

HOMEWORK: SUPPOSE $r_0 = 10\mu, 100\mu$.

① SOLVE FOR A SEMICONDUCTOR AT $T = 4°K$, $300°K$

② SOLVE FOR WATER @ $300°K$

Si $\quad C_p|_{4°K} = 1.68 \times 10^{-6}$ $\frac{\text{JOULE}}{\text{GM}\cdot°K}$

$C_p|_{100°K} = 0.259$

Ge $\quad C_p|_{4°} = 1.44 \times 10^{-5}$ $\frac{\text{JOULE}}{\text{GM}\ °K}$ (CHANGES W/ IMPURITIES)

$C_p|_{100°} = 0.191$

② CASE ②.

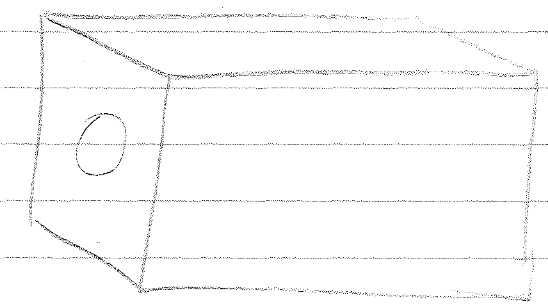
$$\frac{\delta T}{\delta \theta} = 0, \quad \frac{\delta T}{\delta r} \approx 0$$

GIVES

$$\frac{1}{T(z)} \frac{\delta^2 T}{\delta z^2} = -U^2 = \frac{1}{T} \frac{\rho c}{K} \frac{\delta T}{\delta t}$$

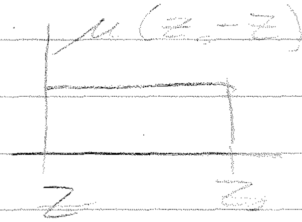
GIVES

$$T(z,t) = A(U) \cos(Uz) e^{-\frac{U^2 K T}{\rho c}}$$



$$T(0,t) = T_0 \, \mu(z_0 - z)$$

(BOUNDARY CONDITION)



$$T(z,t) = \int_0^\infty A(U) \cos Uz \, dU \qquad \text{(FOURIER XFORM)}$$

$$\Rightarrow A(U) = \frac{2}{\pi} \int_0^\infty T(0,z) \cos(Uz) dz$$

$$T(z,t) = \int_0^\infty A(U) \cos(Uz) e^{-\frac{U^2 K T}{\rho c}} dU$$

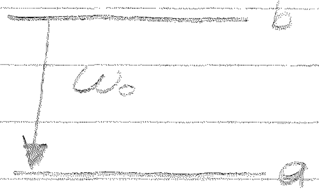
$$= \frac{T_0}{2} \sqrt{\frac{\rho c}{\pi K T}} \int_0^{z_0} dx \left\{ e^{-(x+z)^2 \left(\frac{\rho c}{4Kt}\right)} + e^{-(x-z)^2 \rho c / 4KT} \right\}$$

$$T(z_0) = \frac{2 T_0}{\sqrt{\pi}} \int_0^{z_0 \sqrt{\frac{\rho c}{4KT}}} e^{-U^2} dU = T_0 \, \text{erf}\left(z_0 \sqrt{\frac{\rho c}{4KT}}\right)$$

$$t_{\frac{1}{2}} \approx z_0^2 \rho c / K$$

BEAM

10-31-75 (FRI) 2 STATE QUANTUM SYSTEM



ENERGY LEVELS

$P[\text{IN STATE } b] = b$

EQ. OF MOTION CONTAINED IN

H = HAMILTONIAN

$$\underset{\substack{\uparrow \\ \text{KNOWN} \\ \text{SOLUTION}}}{H = H_0} + \underset{\substack{\uparrow \\ \text{PERTURBATION} \\ \text{(EX. APPLIED E OR LIGHT FIELD)}}}{V}$$

ONE ASSUMES THAT:

H_0 GIVES $\psi = a\,\phi_a\, e^{-i\omega_a t} + b\,\phi_b\, e^{-i\omega_b t}$

$$\phi_a \Longrightarrow |a\rangle$$
$$\phi_b \Longrightarrow |b\rangle$$

$$\int \phi_a^* \phi_b = \underset{\text{BRA}}{\langle a|}\underset{\text{KET}}{b\rangle} = \delta_{ab}$$

$$\psi = a|a\rangle e^{-i\omega_a t} + b|b\rangle e^{-i\omega_b t}$$

ASSUME a & b ARE FUNCTIONS OF TIME

$a = a(t)$ $b = b(t)$

WANNA FIND ψ FOR $H_0 + V$

$E_a = \langle a|\psi_0|a\rangle$

WANNA FIND: $\langle a|H_0 + V|\psi\rangle$

USING $\langle a|b\rangle = 0$

$\langle a|a\rangle = 1$

GIVES

$$\langle a|H_0+V|\psi\rangle = \langle a|H_0|a\rangle a e^{-i\omega_a t} + \langle a|V|b\rangle e^{-i\omega_b t}$$

$$\langle a|H_0|b\rangle = \langle a|E_b|b\rangle = 0$$

SINCE $H\psi = \frac{i}{\hbar}\frac{\partial \psi}{\partial t}$

$$\langle a|H_0|a\rangle a e^{-i\omega_a t} + \langle a|V|b\rangle b e^{-i\omega_b t}$$

$$= i\hbar\left[\dot{a} e^{-i\omega_a t} - i\omega_a a e^{-i\omega_a t}\right]$$

DEFINE: $V_{ab} = \langle a|V|b\rangle$

ASSUME $V_{aa} = V_{bb} = 0$; $V_{ab} = V_{ba}$

b

$\omega_0 = \omega_b - \omega_a$

a

$$V_{ab}\, b\, e^{-i\omega_b t} = i\hbar \dot{a} e^{-i\omega_a t}$$

$$V_{ab}\, a\, e^{-i\omega_a t} = i\hbar \dot{b} e^{-i\omega_b t}$$

EQUIVALENTLY:

$$\left.\begin{aligned} \dot{a} &= -\frac{i}{\hbar} V_{ab}\, b\, e^{-i\omega_0 t} \\ \dot{b} &= -\frac{i}{\hbar} V_{ab}\, a\, e^{i\omega_0 t} \end{aligned}\right\} \text{WANNA SOLVE}$$

$V = eE_0 x_{ab} \cos \omega t \Leftarrow$ APPLIED $\vec{E}$ FIELD

$e\langle a|x|b\rangle = \mu_{ab} \Leftarrow$ DIPOLE

GIVES

$$\dot{a} = \frac{-i}{\hbar} \frac{\mu_{ab}}{2} E_0 b \left[e^{i(\omega-\omega_0)t} + e^{-i(\omega+\omega_0)t} \right]$$

$$\dot{b} = \frac{-i}{\hbar} \frac{\mu_{ab}}{2} E_0 a \left[e^{i(\omega+\omega_0)t} + e^{-i(\omega-\omega_0)t} \right]$$

ASSUME DAMPING:

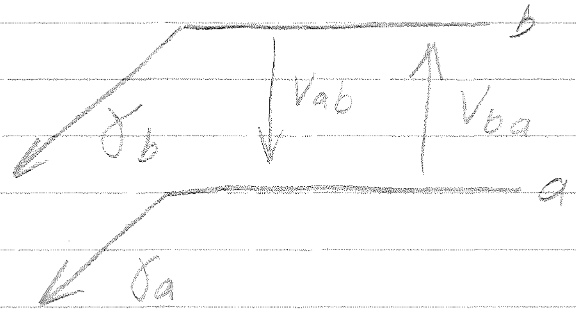
$$\dot{a} = -\frac{\gamma_a}{2} a \qquad \dot{b} = -\frac{\gamma_b}{2} b$$

GIVES:

$$\dot{a} = \frac{-i\mu_{ab} E_0 b}{2\hbar} e^{i\Omega t} - \frac{\gamma_a}{2} a$$

$$\dot{b} = \frac{-i\mu_{ab} E_0 a}{2\hbar} e^{-i\Omega t} - \frac{\gamma_b}{2} b$$

$$\Omega = \omega - \omega_0$$



$$a \sim \alpha e^{-\frac{\gamma_a}{2}(t-t_0)}$$
$$b \sim \beta e^{-\gamma_b/2 (t-t_0)}$$

INITIAL CONDITIONS

1. $\alpha = 1,\ \beta = 0$ @ $t = t_0$
2. $\beta = 1,\ \alpha = 0$ @ $t = t_0$

$$\begin{cases} \dot{\alpha} = -\frac{i\mu E_0}{2\hbar} \beta e^{i\Omega(t-t_0)} e^{\frac{\gamma_a - \gamma_b}{2}(t-t_0)} e^{i\Omega t_0} \\ \dot{\beta} = -\frac{i\mu E_0}{2\hbar} \alpha e^{-i\Omega(t-t_0)} e^{-\left(\frac{\gamma_a-\gamma_b}{2}\right)(t-t_0)} e^{-i\Omega t_0} \end{cases}$$

TO FIRST ORDER IN $\vec{E}$ FIELD

GIVES

$$\beta(t) = \int_{t_0}^{t} \{\dot{\beta}\}\, dt$$

$$= -\frac{i\mu E_0}{2\hbar} e^{-i\Omega t_0} \times \frac{e^{\left[-i\Omega - \frac{\gamma_a}{2} + \frac{\gamma_b}{2}\right](t-t_0)} - 1}{-i\Omega - \frac{\gamma_a}{2} + \frac{\gamma_b}{2}}$$

$$P = \text{POLARIZATION} = \langle \psi | \mu | \psi \rangle$$

$$= \mu \left[a^* b e^{-i\omega_0 t} + a b^* e^{i\omega_0 t} \right]$$

FLUC & CHNG: $\tau = t - t_0$, $\gamma_{ab} = \gamma_a + \gamma_b$

$$P = \mu \left(\frac{-iE_0}{2\hbar} \right) \left\{ \frac{e^{i(\omega t + \Omega\tau)}}{-i\Omega - \frac{\gamma_a}{2} + \frac{\gamma_b}{2}} \times \left(e^{i\Omega - \gamma_a \tau} - e^{-\gamma_{ab}\tau} \right) - \frac{e^{-i\omega t - i\Omega t}}{i\Omega + \frac{\gamma_b - \gamma_a}{2}} \left(e^{[i\Omega - \gamma_a]\tau} - e^{-\gamma_{ab}\tau} \right) \right\}$$

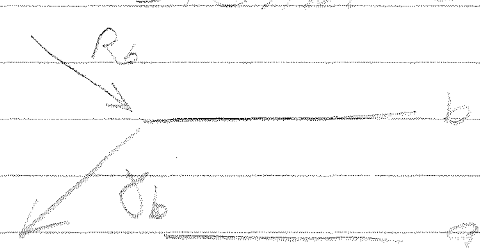
ASSUME $R_a(t) \simeq$ CONSTANT
= RATE @ WHICH ATOMS ARE EXCITED INTO STATE a

ANYWAY, THE ANSWER IS

$$P_x = \frac{\mu^2 E_0}{2\hbar}\left(\frac{R_b n_b}{\gamma_b} - \frac{R_a n_a}{\gamma_a}\right)$$

$$\times \frac{1}{(\omega-\omega_0)^2 + \gamma_{ab}^2}\left[(\omega-\omega_0)\cos\omega t - \gamma_{ab}\sin\omega t\right]$$

= STEADY STATE POLARIZATION



11-3-75 (MON)

$\vec{E}$ FIELD ON 2 STATE SYSTEM

n_a $\quad n_b \Leftarrow$ # ATOMS

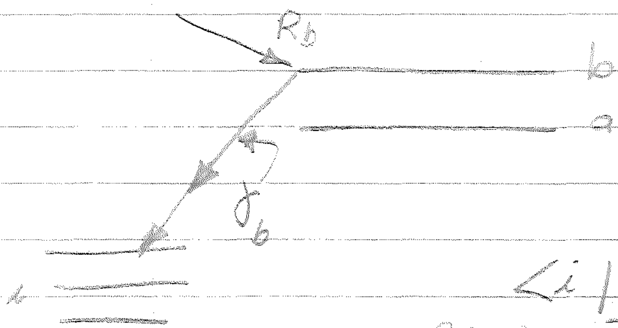
R_a $\quad R_b \Leftarrow$ PUMPING

γ_a $\quad \gamma_a \Leftarrow$ DECAY

YA GET:

$$P = \frac{\mu^2 E_0}{2\hbar}\left[\frac{R_b n_b}{\gamma_b} - \frac{R_a n_a}{\gamma_a}\right]\left[\frac{e^{i\omega t}}{\Omega - i\gamma_{ab}} - \frac{e^{-i\omega t}}{\Omega + i\gamma_{ab}}\right]$$

$$= \frac{\mu^2 E_0}{\hbar}\left(\frac{R_b n_b}{\gamma_b} - \frac{R_a n_a}{\gamma_a}\right)\left[(\omega-\omega_0)\cos\omega t - \gamma_{ab}\sin\omega t\right]$$



$$\langle i|V|b\rangle$$

PROB $i \to b \sim |\langle i|V|b\rangle|^2$

FOR A COLLISION

$\langle$ OUTGOING $|\ V\ |$ INCOMING $\rangle$

$$\langle e^{-ik\cdot x} | V(x) | e^{ik\cdot x} \rangle = \mathcal{F}[V(x)]$$

ANYWAY ASSUMING INDEPENDENCE

P_T = PROB. OF TRANSITION $= \sum_i P_i$

$$= \sum_i |\langle i|V_0|b\rangle|^2$$

DECAY $\frac{\delta n_b}{dt} = P_T\, n_b$

$$\Rightarrow n_b = n_{b_0} e^{-t\gamma_b} \ni \gamma_b = P_T$$

$$\therefore \gamma_b = \sum_i |\langle i|V|b\rangle|^2$$

BOLTZMAN TRANSPORT EQN.

(SEE TEXT) $= \frac{1}{m^*} \vec{\nabla}_v f \cdot \vec{F} + \vec{\nabla}_x f \cdot \vec{v} + \frac{\delta f}{\delta t}$

$$f(\vec{v}, \vec{x}, t) \Rightarrow \frac{\delta f}{\delta \vec{v}} \cdot \vec{a} + \frac{\delta f}{\delta \vec{x}} \vec{V} + \frac{\delta f}{\delta t} = 0$$

$$\frac{df}{dt} = \frac{\delta f}{\delta n} \frac{\delta v}{\delta t} + \frac{\delta f}{\delta x} \cdot \frac{\delta x}{\delta t} + \frac{\delta f}{\delta t}$$

$= 0$ IN AN EQUALIBRIUM

$$\frac{dv}{dx} = a = F/m^*$$

$$\frac{dx}{dt} = V$$

$$f \sim e^{-t/\tau}$$

$$\frac{df}{\delta t} = -f/\tau$$

IN EQUALIBRIUM: $\frac{f_0 - f}{\tau} = \vec{V} \cdot \nabla_x f + a \cdot \nabla_v f$

NOW $p = \hbar k$

IN QM: $\frac{f_0 - f}{\tau} = \frac{p}{m^*} \cdot \nabla_x f + \frac{\vec{F}}{\hbar} \cdot \nabla_k f$

11-7-75 (FRI)

TEST # 2 NEXT WEDNESDAY

MATERIAL IN TEXT: CHAPT 4

$$\frac{f_0 - f}{\tau} = \vec{V} \cdot \nabla_x f + \bar{a} \cdot \nabla_v f$$

APPROXIMATION: $\frac{\delta^2 f}{\delta x \delta v} \approx \frac{\delta^2 f_0}{\delta x \delta v}$

METAL

$$f_0 = n\left(\frac{m}{2\pi kT}\right)^{3/2} e^{-\frac{mv^2}{2kT}} \Leftarrow \text{MAXWELL BOLTZMAN DISTRIBUTION}$$

WILL CALCULATE

① ELECTRON CURRENT DENSITY

② HEAT CURRENT DENSITY

WORK INVOLVES SOLUTION OF

$$I_n = \int_{-\infty}^{\infty} E^n e^{-E/kT} dv_x \quad ; E = \tfrac{1}{2} m v^2$$

$$\mathcal{D}_n = \int_{-\infty}^{\infty} e^{-ax^2} x^n dx$$

(0) $\mathcal{D}_0 = \int_{-\infty}^{\infty} e^{-ax^2} dx$

$$(\mathcal{D}_0)^2 = \int e^{-ax^2} dx \int e^{-ay^2} dy$$

$$x = r\cos\theta \; ; \; y = r\sin\theta$$

$$(\mathcal{D}_0)^2 = \int_0^{\infty} r\,dr \int_0^{2\pi} d\theta\, e^{-ar^2}$$

$$= \pi/a$$

$$\mathcal{D}_0 = \sqrt{\pi/a} \qquad \mathcal{D}_0' = \tfrac{1}{2}\sqrt{\tfrac{\pi}{a}}$$

(1) $\mathcal{D}_1' = \int_0^{\infty} x e^{-ax^2} dx$

$$= \frac{1}{2a} \qquad \mathcal{D}_1' = \frac{1}{2a}$$

$$\mathcal{D}_n' = -\frac{\delta}{\delta a}\left[\int_0^{\infty} e^{-ax^2} x^{n-2} dx\right]$$

$$= -\frac{\delta}{\delta a} \mathcal{D}_{n-2}'$$

$$I_2' = -\frac{\delta}{\delta a} I_0' = \frac{\sqrt{\pi}}{4} a^{-3/2}$$

ETC.

$$I_0' = \frac{1}{2}\sqrt{\pi/a}$$
$$I_1' = \frac{1}{2a}$$
$$I_2' = \frac{1}{4}\sqrt{\pi}\, a^{-3/2}$$
$$I_3' = \frac{1}{2a^2}$$
$$\vdots$$
$$I_n' = \frac{1}{2}\Gamma\left(\frac{n+1}{2}\right) a^{-\frac{(n+1)}{2}}$$

REWRITTING BOLTZMAN EQN: (1-0)

$$f = f_0 - \tau\left(V_x \frac{\delta f_0}{\delta x} + a_x \frac{\delta f_0}{\delta V_x}\right)$$

DEFINE CURRENT DENSITY:

$$J_x = -e \sum V_x$$
$$= -e \int_{-\infty}^{\infty} f\, V_x\, dV_x$$
$$\int f_0(v)\, v\, dV = 0$$
$$= e \iiint_{-\infty}^{\infty} \tau\left(V_x \frac{\delta f_0}{\delta x} + a_x \frac{\delta f_0}{\delta V_x}\right)$$
$$\times V_x\, dV_x\, dV_y\, dV_z$$

THERMAL CURRENT DENSITY:

$$C_x = \iiint_{-\infty}^{\infty} f\, V_x\, \mathcal{E}\, d^3V$$

NOW $\frac{\delta f_0}{\delta x} = \left(\frac{mv^2}{2kT} - \frac{3}{2}\right)\frac{f_0}{T}\frac{\delta T}{\delta x}$

$$\frac{\delta f_0}{\delta V_x}\frac{\delta V_x}{\delta t} \Rightarrow \frac{\delta V_x}{dt} = \frac{eE_x}{m}$$

$$\Rightarrow \frac{\delta f_0}{\delta V_x}\frac{\delta V_x}{\delta t} = \frac{eE_x}{kT} V_x f_0$$

GIVES

$$J_x = \frac{ne\tau k}{m}\frac{\delta T}{\delta x} + \frac{ne^2\tau}{m} E_x$$

$$C_x = \frac{-5nk^2T\tau}{m}\frac{\delta T}{\delta x} - \frac{5nekT\tau E_x}{2m}$$

$\vec{J} = \sigma \vec{E}$ @ $T = 0$ GIVES $\sigma = ne^2\tau/m$

THERMAL CONDUCTIVITY

$$K \equiv \frac{C_V}{\delta T/\delta x}$$

FOR $E_x = 0 \Rightarrow K = \frac{-5nk^2T\tau}{m}$

WIEDEMANN-FRANZ RATIO

$\frac{K}{\sigma T} = \frac{\pi^2}{3}\left(\frac{k}{e}\right)^2$ ⇐ MATERIAL INDEPENDENT.

$\approx 2.5 \times 10^{-8}$

TO GET, USE FERMI-DIRAC

$$f_0 = \frac{1}{1 + e^{E-E_F/kT}}$$

AND GO (ie LOOK IN BOOK)

$$\int_{-\infty}^{\infty} \frac{x^2 e^x}{(1+e^x)^2}\,dx = \frac{\pi^2}{3}$$

END OF MATERIAL COVERED ON TEST #2

9-10-75 (MON.) (GUEST LECTURE)

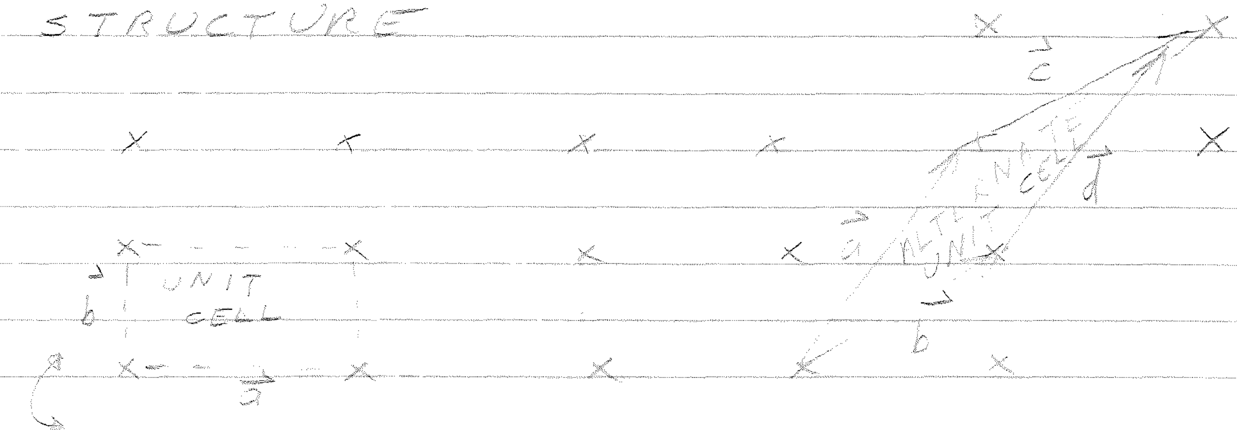
CRYSTAL STRUCTURE

SINGLE CRYSTAL - SAME CRYSTAL STRUCTURE THOUGHOUT

POLY CRYSTALLINE - MANY CRYSTAL STRUCTURES

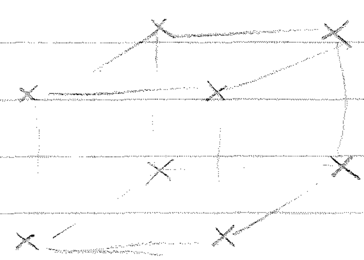
AMORPHOUS - CHANGING CRYSTALLINE STRUCTURE

LIQUID CRYSTAL - TWO DIMENSIONAL CRYSTAL STRUCTURE

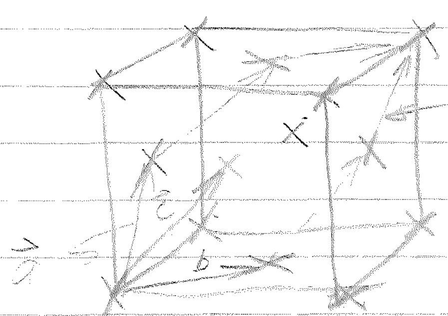


$\vec{r} = r + n_1\vec{a} + n_2\vec{b}$

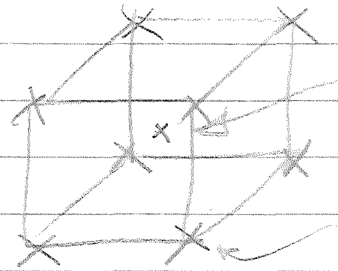
IN 3-D, SIMPLIST IS ON CUBE



FACE CENTERED CUBE



BODY CENTERED CUBIC



EACH ATOM SHARED WITH 8 OTHERS
(SHARING)

nn = NEAREST NEIGHBOR

SO WE GOT	VOLUME	ATOMS / CELL	# nn	DISTANCE
∘ SIMPLE	a^3	1	6	a
∘ BODY CENTER	a^3	2	8	$\sqrt{3}a/2$
∘ FACE-CENTER CUBIC	a^3	4	12	$\frac{a}{\sqrt{2}}$

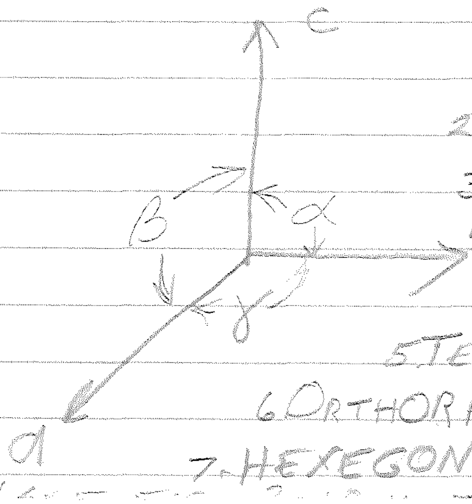
→ NEXT NEAREST NEIGHBOR

nnn	d_{nnn}	EX
12	$\sqrt{2}a$	
6	a	Li, Na K, Cs
6	a	Cu, Au

PARALLEL PIPEDON

BRAVAIS LATTICE - PERIODIC STRUCTURE

DEF: ∞ # PTS. IN SPACE WITH THE PROPERTY THAT THE ARRANGEMENT OF POINTS AROUND A GIVEN PT. IS IDENTICAL WITH THAT ABOUT ANY OTHER POINT.



GET 7 CLASSES

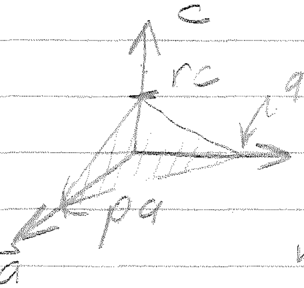
1. CUBIC: $a = b = c$, $\alpha = \beta = \gamma = \pi/2$
2. TRICLINIC: $a \neq b \neq c$, $\alpha \neq \beta \neq \frac{\pi}{2} \neq \gamma$
3. MONOCLINIC: $\alpha = \beta = \frac{\pi}{2} \neq \gamma$, $a \neq b \neq c$
4. RHOMBOHEDRAL: $a = b = c$, $\alpha = \beta = \gamma \neq \frac{\pi}{2}$
5. TETRAGONAL: $a = b \neq c$, $\alpha = \beta = \gamma = \frac{\pi}{2}$
6. ORTHORHOMBIC: $a \neq b \neq c$, $\alpha = \beta = \gamma = \frac{\pi}{2}$
7. HEXEGONAL: $a = b \neq c$, $\gamma = 120°$, $\alpha = \beta = \frac{\pi}{2}$

EACH OF THESE CAN BE PRIMITIVE, BCC, FCC, OR BASE CENTERED ⇒ 

n FOLD ROTATION: MAY ROTATE $\frac{360°}{n}$ AND GET THE SAME THING.

11-14-75 (FRI) (GUEST LECTURE)

MILLER INDICES



DEFINED SPACE LATTICE VIA TRANSLATION VECTOR

$$\vec{T} = n_1\vec{a} + n_2\vec{b} + n_3\vec{c}$$

WISH TO FIND INTEGERS h, k, l SUCH THAT

$$h : k : l = \frac{1}{p} : \frac{1}{q} : \frac{1}{r}$$

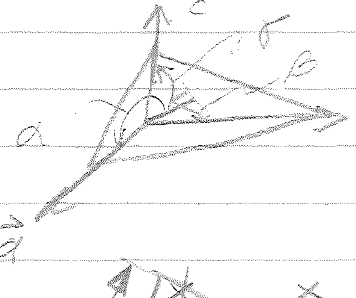
EX: $p = 2,\ q = 3,\ r = 1$

$$\Rightarrow (h, k, l) = (3, 2, 6)$$

FOR NEGATIVE INTERCEPTS, USE $\bar{1}$

IF NO INTERCEPT, USE $0 = \frac{1}{\infty}$

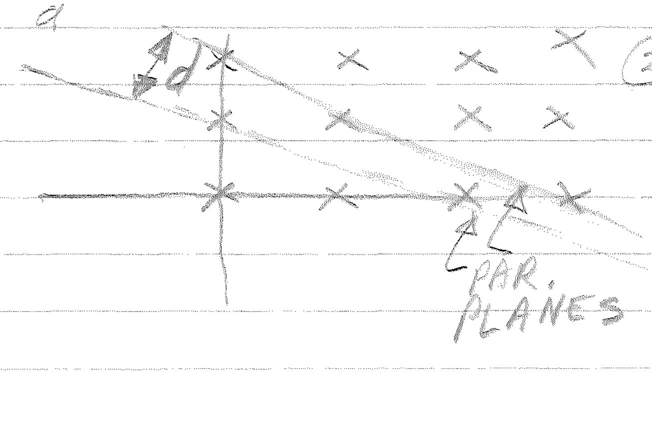
⊥ FROM PLANE TO ORIGIN:



(1) $\cos\alpha : \cos\beta : \cos\gamma$

$$= \frac{1}{pa} : \frac{1}{qb} : \frac{1}{rc}$$

$$= \frac{h}{a} : \frac{k}{b} : \frac{l}{c}$$



(2) $d = \frac{a}{h}\cos\alpha$

$$= \frac{b}{k}\cos\beta$$

$$= \frac{c}{l}\cos\gamma$$

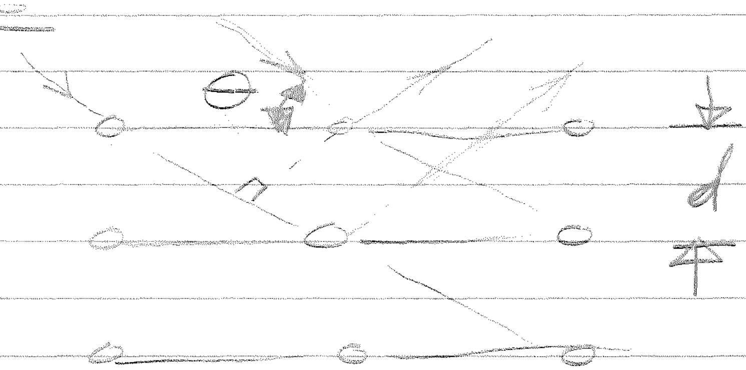
$$\left.\begin{aligned}\cos^2\alpha &= d^2h^2/a^2\\ \cos^2\beta &= d^2k^2/a^2\\ \cos^2\gamma &= d^2\ell^2/a^2\end{aligned}\right\}\ \sum_1^3 \cos^2 = 1$$

$$\Rightarrow \frac{d^2}{a^2}(h^2+k^2+\ell^2) = 1$$

$$\Rightarrow d = \frac{a}{\sqrt{h^2+k^2+\ell^2}}$$

EXPERIMENTAL DETERMINATION
X-RAY DIFFRACTION

(1) BRAGG

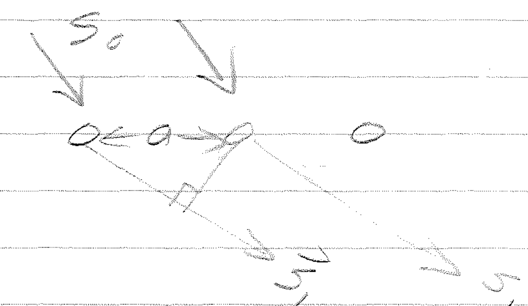


$n\lambda = 2d\sin\theta \leftarrow$ PATH DIFFERENCE

$\lambda \leq 2d$ (SINCE $\sin\theta \leq$

$n = 0, \pm 1, \pm 2, \ldots$

(2) VAN LAUE



$\vec{a}(\vec{S}_1 - \vec{S}_0) = h\lambda$ $h = 0, 1, 2, \ldots$

IN 3-DIMENSIONS:

$\vec{b}(\vec{S}_1 - \vec{S}_0) = k\lambda$

$\vec{c}(\vec{S}_1 - \vec{S}_0) = \ell\lambda$

RECIPROCAL LATTICE

DEFINE $\vec{a}^* = \vec{a} \times \vec{b} \,/\, (\vec{a} \cdot \vec{b} \times \vec{c})$

$$\vec{b}^* = (\vec{c} \times \vec{a}) \,/\, (\vec{b} \cdot \vec{c} \times \vec{a})$$

$$\vec{c}^* = \vec{a} \times \vec{b} \,/\, (\vec{c} \cdot \vec{a} \times \vec{b})$$

PROPERTIES

1. $VOL_{UNIT\ CELL} = 1 / V^*_{UNIT\ CELL}$
2. $\vec{a} \cdot \vec{a}^* = 1$

   $\vec{c} \cdot \vec{c}^* = 1$

   $\vec{b} \cdot \vec{b}^* = 1$
3. $\vec{a} \cdot \vec{b}^* = 0$

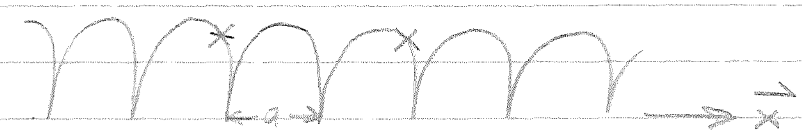
OTHER PROPERTIES

1) $\vec{r}^*(h, k, l)$ IS $\perp$ (h, k, l) LATTICE PLANE
2) $|r^*(h, k, l)| = 1 / d(h, k, l)$
3. RECIPRICAL OF F.C.C. IS B.C.C

11-17-75 (MON) WAVE FUNCTION FOR ELECTRON

$\psi_{\vec{k}}(\vec{x}) = e^{i k \cdot \vec{x}} \; U_{\vec{k}}(\vec{x}) \Leftarrow$ TRUE FOR PERIODIC LATTICE

$U_{\vec{k}}(\vec{x})$ IS PERIODIC = BLOCK FUNCTIONS



① USE PERIODIC PROPERTY

$$|\psi_{\vec{k}}(x)|^2 = |\psi_{\vec{k}}(x + a)|^2$$

$$\psi_{\vec{k}}(\vec{x} + \vec{a}) = e^{i f(\vec{k}, \vec{a})} \psi_{\vec{k}}(x)$$

KINEMATICAL CONSIDERATIONS:

① TRANSLATION

$$\psi(x_0 + x) = \psi(x_0) + \left.\frac{\delta \psi}{\delta x}\right|_{x_0} x + \frac{1}{2!} \left.\frac{\delta^2 \psi(x_0)}{\delta x^2}\right|_{x_0} x^2 + \dots$$

$$\psi(x+x_0) = \psi(x_0) + \frac{\delta \psi(x_0)}{\delta x} x + \frac{1}{2!} \frac{\delta^2 \psi(x_0)}{\delta x^2} x^2$$

$$= e^{x \frac{\delta}{\delta x_0}} \psi(x_0)$$

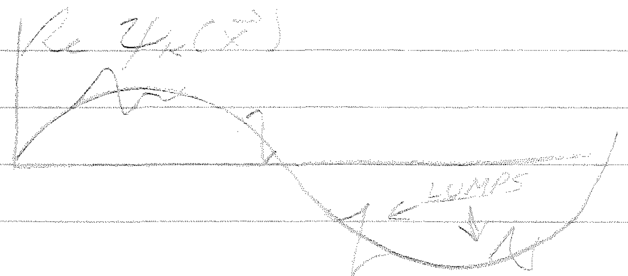
NOW $\frac{\hbar}{i} \frac{\delta}{\delta x} \Leftrightarrow \vec{p} \Leftrightarrow \hbar \vec{k}$

$$\Rightarrow \psi(x+x_0) = \psi(x_0) e^{i x k_x}$$

THUS $f(k, a) = \vec{k} \cdot \vec{a}$

IN 3-D:

$$\psi_{\vec{k}}(\vec{x}) = u_{\vec{k}}(\vec{x}) e^{i \hat{k} \cdot \vec{x}}$$



ABELIAN GROUPS (COMMUTE)
$AB\vec{x} = BA\vec{x}$
$\exists\, N \ni A^N = A \quad (A^{N-1} = 1)$
ONE DIMENSIONAL IRREDUCIBLE REPRESEN.
$\Rightarrow A = e^{i\xi}$

$\vec{k} \cdot \vec{p}$ METHOD

FOR BEHAVIOR OF ELECTRONS (HOLES)

FOR SMALL K,

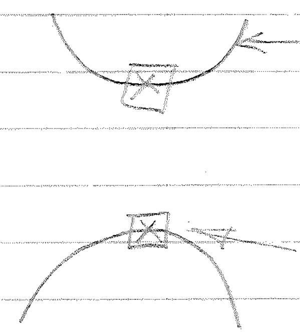
FOR AN ELECTRON:

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V\right] U_{\vec{k}}(\vec{r})\, e^{i\vec{k}\cdot\vec{r}} = E(\vec{k})\, U_{\vec{k}}(\vec{r})\, e^{i\vec{k}\cdot\vec{r}}$$

GRINDING THRU:

$$\left[\frac{\vec{p}^2}{2m} + \frac{\hbar}{m}\vec{k}\cdot\vec{p} + \frac{\hbar^2 k^2}{2m} + V\right] U_{\vec{k}}(\vec{r}) = E(\vec{k})\, U_{\vec{k}}(\vec{r})$$

FOR DIRECT GAP MATERIAL (SMALL K)



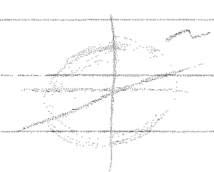
CONDUCTION BAND (IN Ge, SPREADING OF S STATE)

$$U_K = \underset{4}{a_c} U_c + \underset{4}{a_v} U_v$$

1 FUNC 3 FUNC

VALENCE BAND (IN Ge, FROM A P STATE)

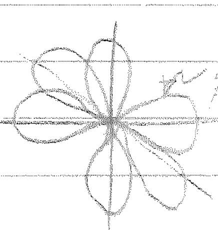
S WAVE FUNCTION



$\sim x^2 + y^2 + z^2$

P STATE FUNCTIONS

3 STATES (6 w/SPIN)



EVEN FUNCTION OF X, Y, Z

$$U_{\vec{k}} = \sum_{i=1}^{4} a_{ki} U_i$$

ASSUME IS SMALL

$$\int U_i^* U_j(r)\, d\vec{r} = \delta_{ij} \leftarrow \text{ORTHONORMAL}$$

THEN

$$E_c U_c + \frac{\hbar}{m}\Big[k_x P_x U_c(\vec{r}) + k_y P_y U_c(\vec{r})$$

$$+ k_z P_z U_c(r)\Big] - E(\vec{k})\, U_c = 0$$

MULTIPLY BY $d\vec{r}$ AND $\int$ GIVES

$$\int U_c^*(\vec{r}) E_c U_c(\vec{r})\, d\vec{r} + \frac{\hbar}{m}\Big[k_x \int U_c^* P_x U_c\, d\vec{r}$$

$$+ k_y \int U_c^* P_y U_c\, d\vec{r} + k_z \int U^* P_z U_z\, d_z\Big]$$

$$- \int U_c^*\ E(\vec{k})\, U(\vec{c})\, d\vec{r}$$

$$= E_c - E(\vec{k}) - \frac{i\hbar^2}{m}\Big[k_x \int U_c^* \frac{\delta U_c}{\delta x}\, \delta \vec{x}$$

$$+ k_y \int U_c^* \frac{\delta U_c}{\delta y}\, dr + k_z \int U_c^* \frac{\delta}{\delta z} U_c\, dr^*$$

DUE TO SYMMERY

$$= -E(\vec{k}) + E_c$$

11-19-75 (WED)

$\vec{K}\cdot\vec{P}$ APPROXIMATION

$U_{\vec{k}} = \sum a_i \, a_{ki} \, U_i(\vec{r})$

$U_c(\vec{r}) \rightarrow$ IN CONDUCTION BAND

$U_v(\vec{r}) \rightarrow$ IN VALENCE BAND

GAVE $0 = \sum_{i=1}^{4} \{ E_i + \frac{\hbar}{m} \vec{k}\cdot\vec{p} - E(k)] a_{ki} V_i(\vec{r})$

USING ORTHOGONALITY OF U_c'S AND U_v'S GIVES FOUR EQUATIONS.

$E - E(\vec{k})(?)$

$$= \int U_c^* E_c U_c + \frac{\hbar}{m} [k_x \int U_c^* P_x U_c + k_y \int y + k_z \int z - \int U_c^* E(\vec{k}) U_c \quad \text{FIRST TERM}$$

$$\int U_c^* E_v U_x d\vec{r} + \frac{\hbar}{m} \{ k_x \int U_c^* P_x U_c d\vec{r} + k_y \int U_c^* P_y U_x d\vec{r} + k_z \int U_c^* P_z U_x d\vec{r} \} - \int U_c^* E(\vec{k}) U_x d\vec{r} \quad \text{SECOND TERM}$$

$$= \frac{\hbar}{m} k_x \int U_c^* P_x U_x d\vec{r}$$

(NOTE: $\int U_c^* P_x U_x d\vec{r} = \int U_c^* P_y U_y d\vec{r}$)

DENOTE: $\frac{\hbar}{m} \int U_c^* P_i U_i = P \Leftarrow$ DIPOLE MOMENT MATRIX ELEMENT

IN SUMMARY, DET. OF a COEFFICIENTS IS:

$$\begin{vmatrix} E_c - E(\vec{k}) & k_x P & k_y P & k_z P \\ k_x P & E_v - E(\vec{k}) & 0 & 0 \\ k_y P & 0 & E_v - E(\vec{k}) & 0 \\ k_z P & 0 & 0 & E_v - E(\vec{k}) \end{vmatrix} = 0$$

PLUGGING ON GIVES:

$$0 = [E_c - E(\vec{k})][E_v - E(\vec{k})]^3 - k_x^2 P^2 (E_v - E(\vec{k}))^2 - k_y^2 P^2 (E_v - E(\vec{k}))^2 - k_z^2 P^2 (E_v - E(\vec{k}))^2$$

SIMPLIFYING:

$$0 = [E_v - E(\vec{k})]^2 \left\{ [E_c - E(\vec{k})][E_v - E(\vec{k})] - k^2 P^2 \right.$$

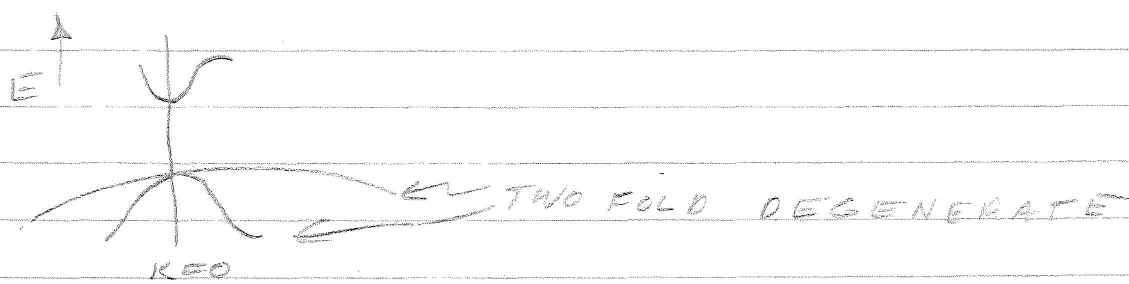
FOUR SOLUTIONS ARE

$$E(\vec{k}) = \begin{cases} E_v \\ E_v \\ \frac{E_c + E_v}{2} + \left[\frac{(E_c - E_v)^2}{4} - k^2 P^2 \right]^{1/2} \\ \frac{E_c + E_v}{2} - \left[\frac{(E_c - E_v)^2}{4} + k^2 P^2 \right]^{1/2} \end{cases}$$

FOR SMALL $\vec{k}$, ONE MAY APPROXIMATE:

$$E(\vec{k}) \simeq E_c \pm \frac{2 k^2 P^2}{E_c - E_v}$$ ← PARABOLIC BAND

"FREE LIKE" FOR SMALL K



OBSERVED IN GERMANIUM

BAND STRUCTURE CALCULATION

HARTREE METHOD

① N ELECTRONS, 1 IN OUTER SHELL
   $V(r) \Leftrightarrow$ N-1 INNER ELECTRONS
② ASSUMED SPHERICAL SYMMETRY
③ REQUIRED SELF CONSISTENCY

CHARGE DENSITY: $\rho = C \sum_{i=1}^{N-1} \psi_i^* \psi_i$

$\Downarrow$

GAVE POTENTIAL $V(\vec{r})$

ASSUME TWO ELECTRONS, $\phi_1(x_1)\phi_2(x_2)$
TO INCLUDE EXCLUSION PRINCIPLE
USE WAVE FUNCTION $\frac{1}{2}\phi_1(x_1)\phi_2(x_2) \pm \frac{1}{2}\phi_1(x_2)\phi_2(x_1)$

EXCHANGE TERM

$$= \frac{1}{2}\begin{vmatrix} \phi_1(x_1) & \phi_2(x_2) \\ \phi_1(x_2) & \phi_2(x_1) \end{vmatrix}$$

IN GENERAL

$$\frac{1}{N!}\begin{vmatrix} \phi_1(x_1 & \phi_2(x_1) & \cdots \\ & & \phi_N(x_N) \end{vmatrix}$$

$\Leftarrow$ ANTI-SYMMETRIZE

CALLED SLATER DETERMINANT

11-21-75 (FRI)

(BAND-STRUCTURE MATERIAL FROM LAST LECTURE IN BOOK)

HARTREE-FOCK APPROACH TO CALCULATING BAND STRUC.

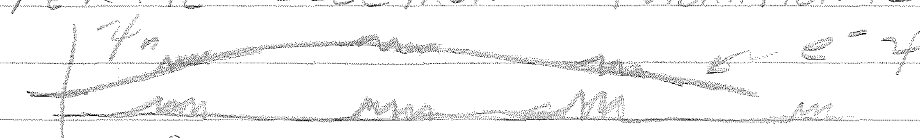
$$H = \underbrace{-\sum_i \frac{\hbar^2}{2M}\nabla_i^2}_{\text{NUCLEUS}}^{(H_n)} \underbrace{- \sum_j \frac{\hbar^2}{2m}\nabla_j^2}_{\text{ELECTRONS}}^{(H_e)} + \underbrace{\frac{1}{2}\sum_{ij}{}' \frac{e^2}{|\vec{r}_i - \vec{r}_j|}}_{\text{ELEC/ELEC TERM}}^{i \neq j}$$

$$+ \underbrace{\frac{1}{2}\sum_{k,l} \frac{Z^2 e^2}{|R_k - R_l|}}_{\text{NUCLEUS-NUCLEUS}} \underbrace{- \frac{1}{2}\sum_{k,j} \frac{Z e^2}{|R_k - \vec{r}_j|}}_{\text{NUCLEUS/ELECTRON}}^{(H_{en})}$$

TOO HAIRY TO SOLVE.

BORN-OPPENHEIMER APPROXIMATION

SEPERATE ELECTRONIC & VIBRATIONAL MOTION



ASSUME $\psi = \psi_e \psi_n$ (NEGLECT H_{en})

GIVES

$$(H_e + H_n)\psi_e \psi_n = E \psi_e \psi_n$$

REFERENCES: ① SLATER,
QUANTUM THEORY OF MOLECULES
AND SOLIDS (II)
② SLATER - QUANTUM THEORY OF MATTER
③ ZIMAN - ELECTRONS AND
PHONONS IN SOLIDS

USING 2nd 3rd & 5TH TERMS HARTREE EQ.

ASSUME $E_e = \int \psi_e^* H \psi_e$

$$= \sum_j \int \phi_j^* \frac{\hbar^2}{2m} \nabla_j^2 \phi_j + \frac{1}{2} \sum_{ij} \int \psi_e^* V_{ee} \psi_e$$

$$\Rightarrow V_{ee} = \frac{1}{2} \sum_{\substack{i \\ i \neq j}} \frac{e^2}{|r_i - r_j|} - \frac{1}{2} \sum_{jk} \frac{e^2}{|R_k - r_j|}$$

$\psi_e = \phi_1 \phi_2 \ldots \phi_j \Leftarrow$ EACH INDIV. e^-

$= \prod_i \phi_i$

INCLUDE SLATER DETERMINANT

$$\psi_e = \frac{1}{\sqrt{N!}} \begin{vmatrix} \phi_i & \cdots \\ \vdots & \end{vmatrix}$$

THE

$$E_e = \sum_j E_j + \frac{1}{2} \sum_j \phi_j^* \phi_i^* V_{ij} \phi_j \phi_i$$

WHERE $V_{ij} = \frac{e^2}{|\vec{r}_i - \vec{r}_j|}$

HARTREE EQN. IS

$$\left\{ H_j + \frac{1}{2} \sum_{i \neq j} \int \frac{e^2}{|r_i - r_j|} \phi_i^* \phi_i \right\} \phi_j = E_j \phi_j$$

IT'S A ONE-ELECTRON EQ.

11-24-75 (MON)

HARTREE-FOCH SUMMARY

WAYS TO DETERMINE ENERGY LEVELS

ASSUME: $\psi = \phi_1(x_1)\phi_2(x_2)\ldots$ ⇐ HARTREE'S ASSUMPTION

ϕ_n = WAVE FNC. OF n^{TH} ELEC.

YOU GET $H\psi = E\psi$

WANNA MINIMIZE USING VARIATION PRINCIPLE

HARTREE-FOCH INCLUDED EXCHANGE TERMS

$$\frac{1}{\sqrt{N!}}\begin{vmatrix} \phi_1(x_1) & \phi_1(x_2) & \ldots \\ \vdots & & \\ & & \ldots\ \phi_n(x_n) \end{vmatrix}$$

FOR TWO ELECTRONS

$$\psi = \frac{1}{2!}\left(\phi_1(x_1)\ \phi_2(x_2) - \phi(x_2)\ \phi_2(x_1)\right]$$

EACH GOT TWO PARTS

$$\phi_1(x_1) = \phi_{1\,SPACE}(\vec{x})\ \phi_{1\,SPIN}(m_{\pm\frac{1}{2}})$$

WISH TO DESYMMITRIZE WAVE FCN.

FOR AN ELECTRON $\psi = [\phi_{1\,SPACE}(x_2)\ \phi_{2\,SPACE}(x_1) + \phi_{1\,SPACE}(x_1)\ \phi_{2\,SPACE}(x_2)[\phi_{1\,SPIN}(1)\,\phi_{2\,SPIN}(2)$

$$- \phi_{1\,SPIN}(2)\ \phi_{2\,SPIN}(1)]$$

ELEC 1 POSITION 2

RESULTING ENERGY IS

$$E = \sum_i \int \phi_i^* \left(-\frac{\hbar^2}{2m}\nabla_i^2\right)\phi_i$$

POT. EN.

$$+ \sum_{i,j}\int \phi_i^*(x_1)\,\phi_j^*(x_2)\left[\frac{e^2}{4\pi\epsilon|x_i - x_j|}\right]$$

$$\times\left[\phi_i(x_1)\,\phi_j(x_2) - \delta_{m_{SPIN\,i},\,m_{SPIN\,j}} \times \phi_i(2)\,\phi_j(1)\right]\ dx_2\,dx_1$$

HOMEWORK PROBLEM: DESCRIBE IN ONE OR TWO PAGES A METHOD OF ENERGY BAND STRUCTURE CALCULATION.

EX: 1. LCAO ⇒ LINEAR COMBINATION OF ATOMIC ORBITALS
2. ORTHOG. PLANE WAVE (OPW)
3. W-S CELLULAR (WIGNER-SEITZ)
4. X-α METHOD, 5. TIGHT BINDING APPROXIMATION

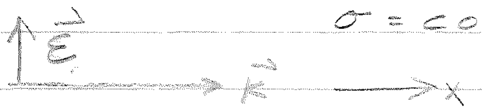
POINT OUT

a. APPLICABILITY AND WHY & WHAT

b. OPTIONAL PROBLEM: WHAT IS THE PHYSICAL SIGNIFICANCE OF THE EXCHANGE TERM? (HINT: PAULI EXCLUSION PRINCIPLE) LOOK AT TWO ELECTRON WAVE FUNCTION.

ABSORBTION OF LIGHT IN SOLID

MAXWELL'S EQN.'S



σ = CONDUCTIVITY

μ = PERMITTIVITY = 1

GIVES ϵ = DIELECTRIC CONST.

$$\frac{\delta^2 E}{\delta x^2} - \frac{\epsilon}{c^2}\frac{\delta^2 E}{\delta t^2} = \frac{4\pi\sigma}{c^2}\frac{\delta E}{\delta t}$$

(OPTIONAL HOMEWORK → DERIVE IT)

ASSUME $E = A e^{i(kx-\omega t)}$

YOU GET

$$\frac{k^2}{\omega^2} = \frac{\epsilon}{c^2} + \frac{i\,4\pi\sigma}{\omega c^2} = \frac{1}{(V^*)^2}$$

REFRATIVE INDEX $(\sigma = 0)$; $r = \sqrt{\epsilon}$

IMAGINARY TERM DESCRIBES ABSORBTION

$$r^* \triangleq c/v^* \quad \text{(COMPLEX DIELECTRIC CONST ?)}$$
$$= \left[\epsilon + i4\pi\sigma/\omega\right]^{1/2}$$
$$= r(1 + i\gamma) = \text{INDEX OF REFRACTION}$$

GIVES $\mathcal{E} = A e^{-\frac{\omega}{c} r \gamma x} e^{i(kx - \omega t)}$

REFR. INDEX

$$r = \frac{1}{\sqrt{2}} \left[\epsilon + \left(\epsilon^2 + \frac{16\pi^2 \sigma^2}{\omega^2} \right)^{\frac{1}{2}} \right]^{\frac{1}{2}}$$

$$\gamma = \left[1 - \epsilon / r^2 \right]^{1/2}$$

HOMEWORK: WHAT IS σ FOR $|r^*|$ TO VARY FROM r BY $> 10\%$. GIVE ANSWER IN $(\Omega\text{-cm})^{-1}$ WITH $\lambda = 5000\,\text{Å}$. ANSWER IS $4000/\Omega\text{cm}$

$dI = -\alpha(1-R) I\,dx \Leftarrow$ ASSUME

$\alpha = \frac{2\omega}{c} r\gamma \Leftarrow$ ABSORBTION $= \gamma$

$= \frac{4\pi}{cr} \sigma$

r_1^*	r_2^*

MAXWELL'S EQN'S GIVE

$$\mathcal{E}_y = A e^{i\omega(r_1^* \frac{x}{c} - t)}$$

$$H_z = A r_1 e^{i\omega(r_1^* \frac{x}{c} - t)}$$

REFLECTED LIGHT =

ASSUME TRANSMITTED LIGHT

$$E_y = A'' e^{i\omega(r_2^* \frac{x}{c} - t)}$$

$$H_z = A'' r_2^* e^{i\omega(r_2^* \frac{x}{c} - t)}$$

SHOW R = REFLECTION COEFFICIENT =

$$= A'A'^* / AA^* = \frac{(r_2 - r_1)^2 + (r_2\gamma_2 - r_1\gamma_1)^2}{(r_2 + r_1)^2 + (r_2\gamma_2 + r_1\gamma_1)^2}$$

$\frac{A'}{A} = r_2 - r_1 / (r_2 + r_1)$

SPECIAL CASES: ① $\sigma = 0$, IN BOTH $r = ?$ 1.5 (n_1, n_2)

② VACUUM METAL INTERFACE

CALCULATE REFLECTION COEFF.

FOR METAL, $R \simeq 1 - 2 / \sqrt{2\pi\sigma/\omega}$

THIS PAGE INTENTIONALLY LEFT BLANK

11-26-75 (WED)

ELECTRON GAS w/ E.M. FIELD FREQ OF ω

$$m_e^* \frac{dv}{dt} + \frac{m_e^* v}{\tau} = -e\mathcal{E} e^{-i\omega t}$$

SOLVING

$$V = -\frac{e}{m^*} \frac{\mathcal{E} e^{-i\omega t}}{\frac{1}{\tau} - i\omega}$$ τ = SCATTERING TIME

CURRENT DENSITY: $J = \sigma \mathcal{E} = neV$

n = # OF ELECTRONS / cm^3

GIVES:

$$\sigma^* = \frac{ne^2}{m^*}\left(\frac{\tau}{1+\omega^2\tau^2} + i\frac{\omega\tau^2}{1+\omega^2\tau^2}\right)$$

$$= \sigma - \frac{i\omega}{4\pi}\epsilon_R$$

$\epsilon_e \Leftarrow$ ELECTRONIC CONTRIBUTION

$$\sigma^* = -\frac{i\omega}{4\pi}\epsilon_e^*$$

$\epsilon_e \Leftrightarrow$ LATTICE

$$\epsilon = \epsilon_L - 4\pi ne^2/m_e^* \left\langle \frac{\tau^2}{1+\omega^2\tau^2} \right\rangle$$

$\langle \cdot \rangle \Leftarrow$ AVERAGING OVER ENERGY

$$\sigma(\omega=0) = ne^2\tau / m_e^*$$

$\alpha = \frac{4\pi}{cr}\sigma$; ABSORPTION: $e^{-\alpha x}$

GET: $\alpha = [ne^3\lambda^2/(\pi m_e^{*2} rc^3)]\langle\tau\rangle^2$

$r\lambda = c$

$$\alpha = (\quad)\frac{n}{\omega^2\langle\tau\rangle^2}$$

12-1-7

SECOND TEST AVERAGED IN THE 50'S

REFLECTIVITY OF A METAL

$$R \simeq 1 - \sqrt{\frac{2\omega}{\pi\sigma}} \quad \text{FOR HI } \omega$$

$$\sigma = \frac{ne^2}{m_e^*}\left\langle \frac{\tau}{1+\omega^2\tau^2} \right\rangle_E$$ ← AVERAGING OVER ENERGY

$$\sigma(\omega \to 0) = \frac{ne^2\langle\tau\rangle}{m_e^*}$$

m_e^* = EFFECTIVE MASS OF ELECTRON

α = ABSORPTION COEFFICIENT (~BEER'S LAW)

$$= \sqrt{\frac{8\pi}{c^2}}\,(\sigma_o\omega)^{1/2}$$

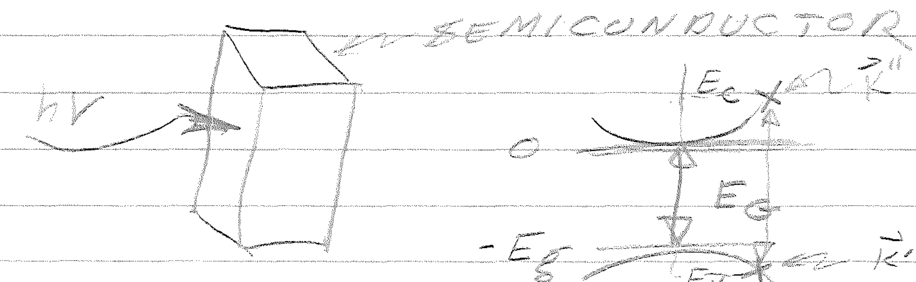
$\omega\tau \ll 1$ FOR A METAL (LOTTA FREE ELEC)

$\omega\tau \gg 1$, $\sigma = \frac{ne^2}{m_e^*\omega}\left(\frac{1}{\tau}\right)$ (SEMICONDUCTOR / INSULATOR)

$$\alpha = \frac{ne^3\lambda^2}{\pi m_e^* r c^3\langle\tau\rangle}$$

r = REAL PART OF REFRATION INDEX

BAND TO BAND TRANSITION



ASSUME NONDEGENERACY OF VALENCE BAND

$$E_v(\vec{K}') = -E_G - \frac{\hbar^2}{2m_h^*}K'^2$$

$$E_c(\vec{K}'') = \hbar^2 K''^2 / (2m_e^*)$$

FROM ENERGY CONSERVATION:

$$\hbar\omega = E_c(\vec{K}'') - E_v(\vec{K}')$$

TRANSITION PROBABILITY

MATRIX ELEMENTS:

$$H_0'(\vec{r})\cos\omega t = \frac{1}{2}H_0'(r_0)\left[e^{i\omega t} + e^{-i\omega t}\right]$$

(CONT.)

MATRIX ELEMENT

$$\int_{\substack{\text{UNIT}\\\text{CELL}}} \psi_m^* H_0(\vec{r})\, \psi_0$$

ψ_0 = VALENCE BAND WAVE FUNCTION

$$= \frac{1}{\sqrt{N}} \underbrace{U_v(\vec{r}, \vec{k}')}_{\text{PERIODIC}} e^{i\vec{k}'\cdot\vec{r}}$$

ψ_m = CONDUCTION BAND WAVE FUNCTION

$$= \frac{1}{\sqrt{N}} U_c(\vec{r}, \vec{k}'') e^{i\vec{k}''\cdot\vec{r}}$$

$U \Leftarrow$ BLOCH FUNCTIONS

MOMENTUM OPERATOR: $P \Leftrightarrow i\hbar\vec{\nabla}$

WE MUST ADD A TERM FOR APPLIED H FIELD

$\vec{\nabla}\times A = \vec{H}$, $\nabla\cdot \vec{A} = 0$; A = MAGNETIC POTENTIAL

$$\Rightarrow \vec{P} = i\hbar\vec{\nabla} + \frac{eA}{c}$$

$$\frac{P^2}{2m} = \frac{-\hbar^2}{2m}\nabla^2 + \underbrace{\frac{i\hbar e}{mc}\vec{A}\cdot\vec{\nabla}}_{\text{PERTURBATION}} + \underbrace{\frac{e^2|A^2|}{2mc^2}}_{\text{ITTY BITTY}}$$

$$H'(\vec{r}) = \frac{i\hbar e}{mc}\vec{A}\cdot\vec{\nabla}$$

GOOD IF $A\cdot\nabla \gg |A^2|$

NOW, $\vec{A} = \hat{a}_0 A \cos(\vec{K}\cdot\vec{r} - \omega t)$

$$= \frac{1}{2} A \hat{a}_0 \left[e^{i(\vec{K}\cdot r - \omega t)} + e^{-i(\vec{K}\cdot r - \omega t)} \right]$$

USUALLY $|\vec{K}| = \frac{\omega r}{c}$ $\ni r = Re(n^*)$

$H'(\vec{r})$ = FERMI POTENTIAL

$$= \frac{ie\hbar}{2mc} A\, e^{i(\vec{k}\cdot\vec{r} - \omega t)}\hat{a}_0\cdot\vec{\nabla} + \text{C.C.}$$

COMPLEX CONJUGATE

RATE OF TRANSITION

$$P \propto \frac{4\,|H_{K'K''}|^2 \sin^2\left[(E_{K''}-E_{K'}-\hbar\omega)\frac{t}{2\hbar}\right]}{(E_{K''}-E_{K'}-\hbar\omega)^2}$$

MATRIX ELEMENT

$$H_{K''K'} = \frac{ie\hbar A}{2Nmc}\int_{\substack{\text{ALL}\\ \text{STATES}}} U_c^*(\vec{r},\vec{k}'')\,e^{-i\vec{k}''\cdot\vec{r}} \times \left[e^{i\vec{K}\cdot\vec{r}}\,\hat{a}_0\cdot\vec{\nabla}\right] U_v^*(\vec{r},\vec{k}')\,e^{i\vec{k}'\cdot\vec{r}}\,d^3r$$

$$= \frac{ie\hbar A}{2Nmc}\int U_c^*(\vec{r},\vec{k}'')\left[\hat{a}_0\cdot\vec{\nabla}U_v(\vec{r},\vec{k}) + i(\vec{a}_0\cdot\vec{k}')\,U_v(\vec{r},\vec{k})\right]e^{i(\vec{k}'+\vec{K}-\vec{k}'')\cdot\vec{r}}\,d^3r$$

ALLOWED DIRECT TRANSITION

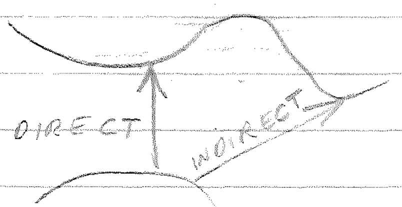
FORBIDDEN DIRECT TRANS

NOW $U_c(r,k) \perp U_v(r,k)$

& $K''-K' \approx$ IS SMALL

$$\Rightarrow \int U_c U_v^*\,d^3r = 0$$

$$\int U_c U_v^* e^{i\epsilon} \simeq 0$$



CHANGE INTEGRAL OVER JUST UNIT CELL, THEN SUM UP CRSYSTALS. GET

$$H_{K''K'} = \sum_{j=1}^{N} e^{i(\vec{k}'+\vec{K}-\vec{k}'')\cdot\vec{R}_j}\int_{\substack{\text{UNIT}\\ \text{CELL}}}[\quad]\,d^3r$$

NON-ZERO ONLY FOR $\vec{K}'+\vec{K} = \vec{K}''$

THEN $H_{K''K'} = N\int_{\substack{\text{UNIT}\\ \text{CELL}}}[\quad]\,d^3r$

12-3-75 (WED)

TRANSITION PROB. IN SEMICONDUCTOR

$$H_{K''\to K'} = \frac{ie\hbar A}{2mc}\int_{\text{UNIT CELL}} U_c^*(\vec{r}, \vec{K''})$$

$$\times\left[\underbrace{\hat{a}_0\cdot\nabla U_v(\vec{r},\vec{K'})}_{\text{ALLOWED}} + \underbrace{i(\hat{a}_0\cdot K')\,U_v(\vec{r},K')}_{\text{SMALL}\sim 0}\right] d^3r$$

CALLED FORBIDDEN TRANSITION

$$H^{\text{ALLOWED}}_{K'',K'} = -\frac{eA}{2mc}\left(\hat{a}_0\cdot\vec{P}_{K'',K'}\right)$$

$$\vec{P}_{K''K'} = -i\hbar\int_{\text{CELL}} U_c(\vec{r},K'')\,\vec{\nabla} U_v(\vec{r},\vec{K'})\,d^3\vec{r}$$

(MUST USE DENSITY OF STATES NOW)

RECALL $P = -i\hbar\vec{\nabla}$

ASSUME MONOCHROMATIC INCIDENCE

USE DENSITY OF STATES $\frac{1}{4\pi^3}$ INTEGRATE OVER K

$$\text{TRANSITION PROBABILITY} = P(E)\,t = \frac{e^2A^2}{4\pi^3 m^2c^2}\qquad \frac{t}{2\hbar}$$

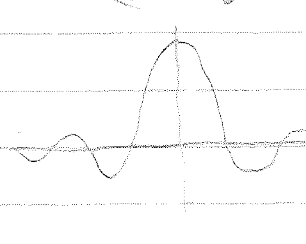
$$\times\int\left|\hat{a}_0\cdot P_{K'',K'}\right|^2\frac{\sin^2\left[(E_{K''}-E_{K'}-\hbar\omega)\frac{t}{2\hbar}\right]}{(E_{K''}-E_{K'}-\hbar\omega)^2}\,d^3K'$$

IN SPHERICAL COORDINATES

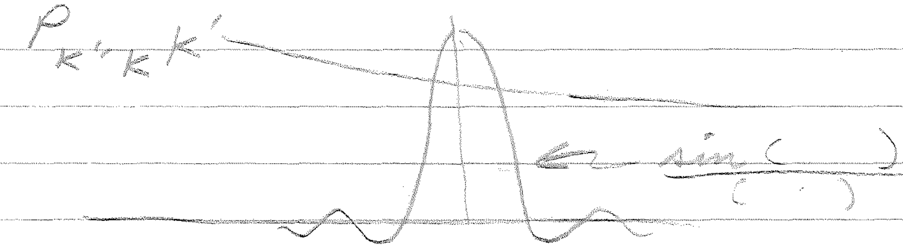
$$d^3K' = K'^2\,dK'\,d\Omega$$

$$\int\left|\hat{a}_0\cdot\vec{P}_{K'',K}\right|^2 d\Omega = 4P\,\overline{P_{K'',K'}}^{\,2}$$

$$P(E)\,t = \frac{e^2A^2}{(\pi mc)^2}\int\overline{P}^{\,2}_{K'',K'}\,\frac{\sin^2\left[(E_{K''}-E_{K'}-\hbar\omega)\frac{t}{\hbar\omega}\right]}{\left[E_{K''}-E_{K'}-\hbar\omega\right]^2}\,K'^2\,dK'$$



9C



SO TO GOOD APPROXIMATION MAY TAKE $P_{K'',K}K'$ TERM OUTSIDE INTEGRAL.

DEFINE $m_r^* = \frac{m_e m_h}{m_e + m_h}$

$$K_0 \ni \hbar\omega = E_G + \frac{\hbar^2 K_0^2}{2m_r^*}$$

$$\Rightarrow K_0 = \frac{\sqrt{2m_r^*}}{\hbar}\sqrt{\hbar\omega - E_G}$$

PUT INTO INTEGRAL SUBJECT TO EARLIER RESTRICTIONS. (SIMILAR TO PREVIOUS HOMEWORK) YA GET

$$P(E) = \frac{e^2 A^2 \sqrt{2m_r^*}}{4\pi m^2 c^2 \hbar^4} \overline{P_{K''K'}}^2 \sqrt{\hbar\omega - E_G}$$

MUST RELATE THIS PROBABILITY TO AN ABSORBTION COEFFICIENT

$\#$ OF INCIDENT PHOTONS $= \frac{|\vec{S}|}{\hbar\omega}$

$\vec{S}$ = POYNTING VECTOR

NUMBER OF ABSORBED PHOTONS $= e^{-\alpha d} \times$ $\#$ OF INC. PHOTONS

d = THICKNESS OF MATERIAL

FOR $\alpha d \ll 1$

$$P(E)\,\hbar\omega/|\vec{S}| = \alpha$$

NOW $\vec{S} = \frac{c}{4\pi}\vec{E}\times\vec{H}$ (FROM FIELD THEORY)

$$= A^2 K \omega / 8\pi \qquad \Rightarrow K = K_{PHOTON}$$

$$\nabla \times \vec{A} = \vec{H}$$

$f_{K''K'}$ = OSCILLATOR STRENGTH

$$= \frac{2\,|P_{K''K'}|^2}{m\hbar\omega}$$

THEN

$$\alpha_{\substack{\text{ALLOWED}\\ \text{DIRECT}\\ \text{ABSORPTION}}} = \frac{2\times 10^5}{r}\left(\frac{2m_r^*}{m}\right)^{3/2} f\,(\hbar\omega - E_G)^{\frac{1}{2}}$$

(IN UNITS OF 1/LENGTH)

APPROXIMATION IN SEMICONDUCTOR IS

$$f \simeq 1 + \frac{m_e}{m_h^*} \Rightarrow$$ SEMICONDUCTOR VALENCE TO CONDUCTION BAND TRANSITION

REFERENCE: R.A. SMITH: WAVE MECHANICS OF CRYSTALLINE SOLIDS

FOR FOBIDDEN

$$f' = \left|\int_{\substack{\text{UNIT}\\ \text{CELL}}} U_c^*(\vec{r},\vec{k}'')\,U_v(\vec{r},\vec{k}')\,d^3r\right|^2$$

$$P(E) = \frac{e^2A^2\,(2m_r^*)^{5/2}}{12\pi m^2\hbar^4}\,(f')\,(\hbar\omega - E_G)^{3/2}$$

$$\alpha_{FORBIDDEN} = 1.8\times 10^5\left(\frac{2m_r^*}{m}\right)^{5/2}\frac{f'}{r}$$

$$\times \frac{1}{\hbar\omega}(\hbar\omega - E_G)^{3/2}$$

FOR ALLOWED

$m_r^* \simeq \frac{m}{2}$, $r=4$, $f=1$, $\hbar\omega - E_G = 0.01\,eV$

$\Longrightarrow \alpha_{ALLOWED} \lesssim 7 \times 10^{-3}/cm$

SAME VALUES WITH

$f' = 0.1$, $\hbar\omega = 1\,eV$

$\Longrightarrow \alpha_{FORBIDDEN} \simeq 5/cm$

IN SOLVING f'

$$U_v(\vec{r}, \vec{k}') \simeq U_v(\vec{r}, \vec{k}'') + \vec{K} \cdot \nabla_K U_v \Big|_{K''} + \frac{K^2}{2!} \nabla^2 (\;) + \dots$$

WILL GIVE A ZERO IN INTEGRAL DUE TO ORTHO.

12-5-75 (FRI)

HOMEWORK (DUE FRIDAY):

1. DERIVE THE EBERS-MOLL EQUATION FOR CURRENT FLOW IN A TRANSISTOR
2. EXPLAIN THE DERIVATION IN PHYSICAL TERMS
3. WHY DOESN'T CURRENT LEAVE (ENTER) AT THE BASE?

ABSORPTION COEFFICIENTS

DIRECT ALLOWED TRANSISION

$$\alpha \sqrt{\hbar\omega - E_G}$$

DIRECT FORBIDDEN TRANSITION

$$\frac{1}{\hbar\omega}\left(\hbar\omega - E_G\right)^{3/2}$$

INDIRECT TRANSITIONS

ONLY FOR − SIGN

ALLOWED:

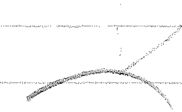
$$\frac{\left(\hbar\omega \pm \hbar\omega_{PHONON} - E_G\right)^2 e^{\hbar\omega_{PH}/kT}_{(-)}}{\left(e^{\frac{\hbar\omega_{PHO}}{kT}} - 1\right)}$$

FORBIDDEN:

$$\frac{\left(\hbar\omega \pm \hbar\omega_{PHONON} - E_G\right)^3 e^{\frac{\hbar\omega_{PH}}{kT}}}{e^{\frac{\hbar\omega_{PHON}}{kT}} - 1}$$

$$\vec{k}_{VAL} = \vec{K}_{PHO} + \vec{k}_{COND}$$

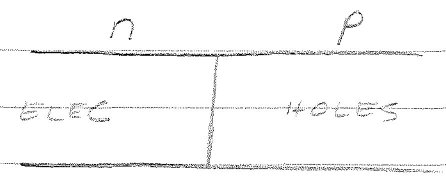
INDIRECT TRANSITION



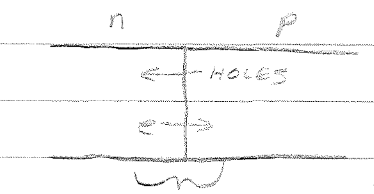
OPTIONAL PROBLEM: FIND ARGUMENT FOR ABSORPTION RELATION W/O HAIRY Q.M. (DENSITY OF STATES AND OCCUPANCY)

(GOOD QUAL QUESTIONS TO FOLLOW)

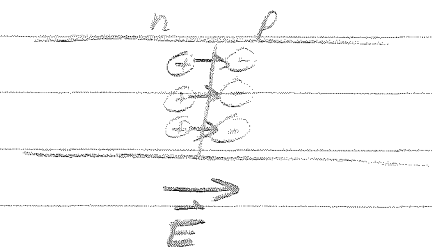
① P-N JUNCTION



CHARGE NUETRALITY IN BOTH JUNCTION.
WHEN YA BRING EM TOGETHER:

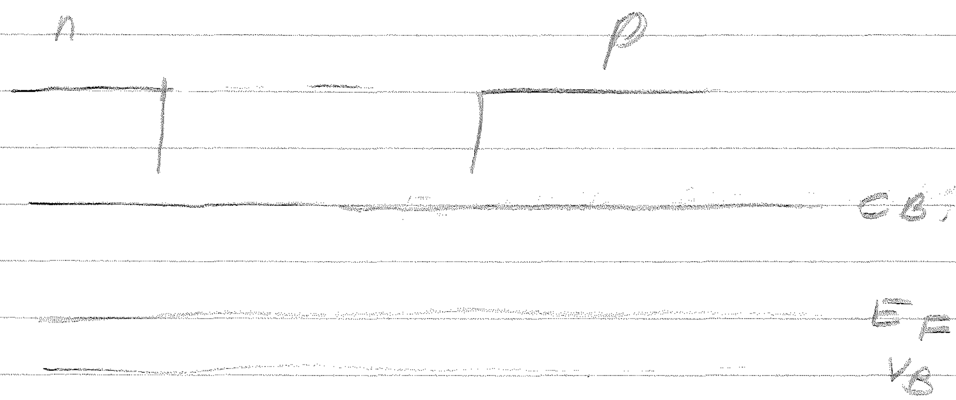


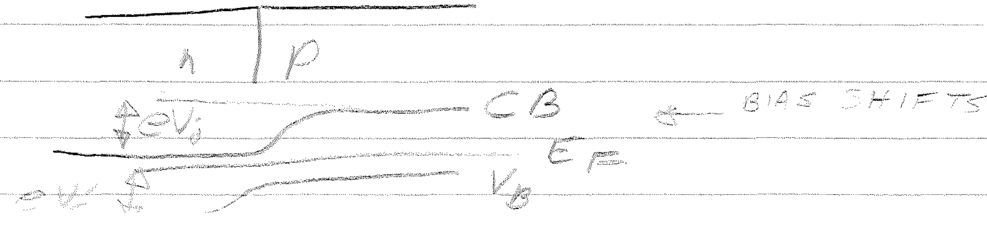
$J = 0 = (\ )\nabla n(x) + (\ )E$



AFTER A FEW MICROSECONDS

$E = f(N_D^+, N_A^-)$
$= f\{$IONIZED DONORS & ACCEPTORS$)$





$$n_p = n_n e^{-eV_i/KT}$$

FOR BIAS

$$n_p = n_n e^{-(e(V_i+V)/KT)}$$

SIMILARLY

$$p_n = p_p e^{-e(V_i+V)/KT}$$

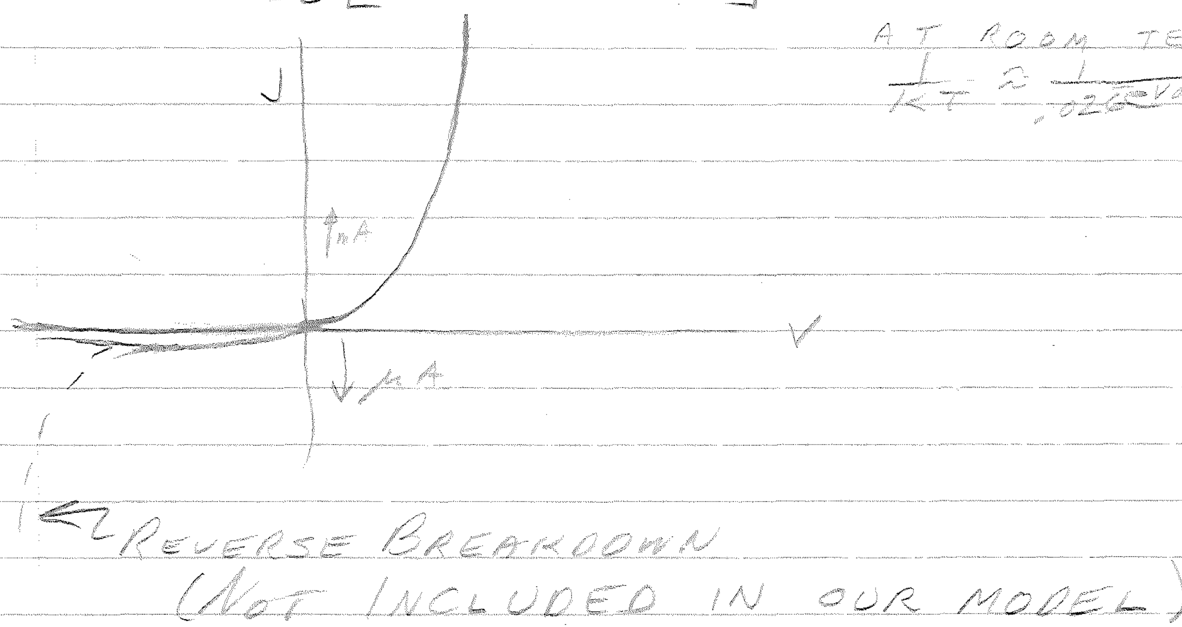
$$J = (\text{CONST})(n_p + p_n) + (n_n + p_p)$$

$$= (\text{CONST})'\left[(n_n + p_p)e^{-eV/KT} - (n_n + p_p)\right]$$

$$= J_{SO}\left[e^{qV/KT} - 1\right]$$

AT ROOM TEMP:

$$\frac{1}{KT} \cong \frac{1}{.026 \text{ VOLTS}}$$



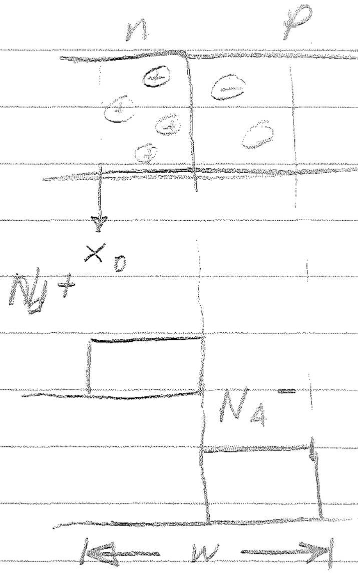
MODELING IN A LINEAR REGION

$$J = J_{s0}\left[1 + \frac{qV}{kT} + \frac{1}{2}\left(\frac{qV}{kT}\right)^2 + \ldots - 1\right]$$

ASSUME $\frac{qV}{kT} \ll 1$

$$J = \frac{qV J_{s0}}{kT}$$

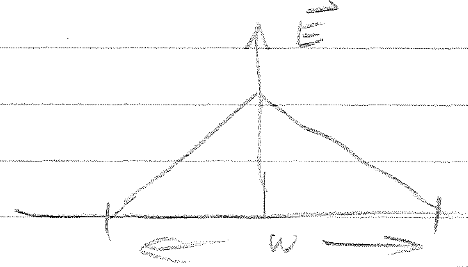
COMPUTATION OF JUNCTION VOLTAGE



N_d^+ = IONIZED DONAR ATOMS

N_A^- = IONIZED ACCEPTOR

USE GAUSS'S LAW: $\nabla \cdot \vec{D} = 4\pi\rho$



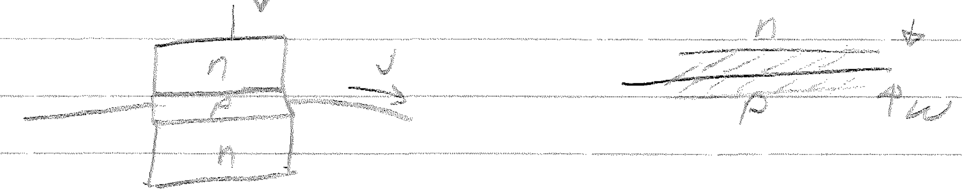
$$w = x_d + x_a = \sqrt{\frac{2\epsilon kT}{q^2}\left(\ln\frac{N_d N_a}{n_i^2}\right)\left(\frac{1}{N_A} + \frac{1}{N_D}\right)}$$

$$V_j = \frac{kT}{e}\ln\left(\frac{N_A N_D}{n_i^2}\right)$$

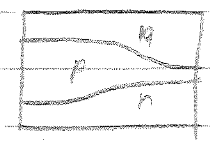
$$w = \left[\frac{2\epsilon V_j}{e}\left(\frac{N_a + N_D}{N_a N_D}\right)\right]^{1/2} \approx \sqrt{V_j}$$

$$w(V) = \text{const}\sqrt{V}$$

$w(V) \approx \sqrt{V}$



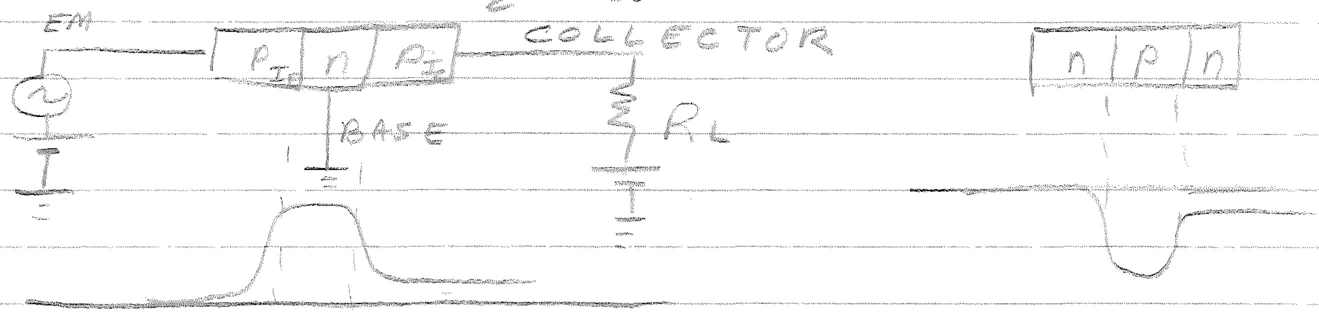
OPERATING PRINCIPLE OF FET TRANSISTOR DEVICES LOOK MORE LIKE (IN EQUALIBRIUM)



12-8-75 (WED)

TRANSISTOR

COMMON BASE CONFIGURATION



INPUT IMPEDANCE, R_{IN}, IS SMALL COMPARED WITH R_{LOAD}

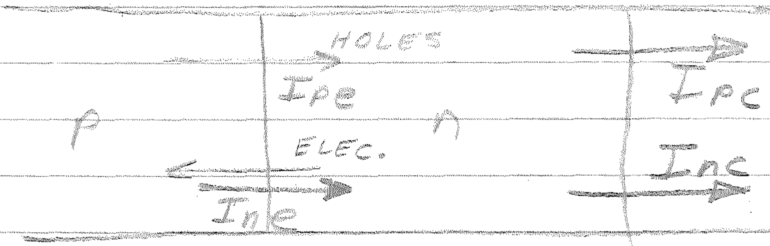
$I_E \sim I_C$

POWER GAIN $\sim \left(\dfrac{I_E^2 R_{IN}}{I_C^2 R_{LOAD}} \right)^{-1} \sim \dfrac{R_{LOAD}}{R_{IN}}$

COMMON BASE

α = CURRENT GAIN

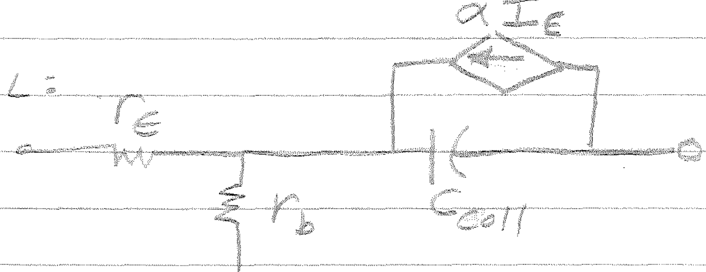
= FRACTION OF COLLECTOR CURRENT MOVING ACROSS EMITTER JUNCTION



$I_{ne} << I_{pe}$ $\quad$ $I_{nc} << I_{pc}$

i.e. I_{ne}, I_{nc} SMALL W.R.T. I_{pc}

MODEL:



P.N. JUNCTION:

$$J = q\left[\frac{D_p p_{no}}{L_p} + \frac{D_n}{L_n} n_{po}\right]\left[e^{\frac{qV}{kT}} - 1\right]$$

WHERE

D_n = DIFFUSION CONSTANT FOR ELECTRONS

D_p = " " " HOLES

L_n = MEAN FREE PATH FOR ELECTRONS (DIFFUSION LENGTH)

L_p = FOR HOLES

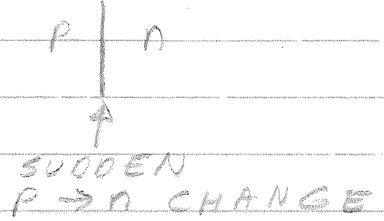
p_{no} = EQUALIBRIUM CONCENTRATION OF HOLES ON n SIDE

n_{po} = FOR ELECTRONS ON p SIDE

$p = p_n e^{qV_s/kT}$ ← BOLTZMAN APPROX.

ASSUMPTIONS:

① "ABRUPT" DEPLETION LAYER ASSUMPTION



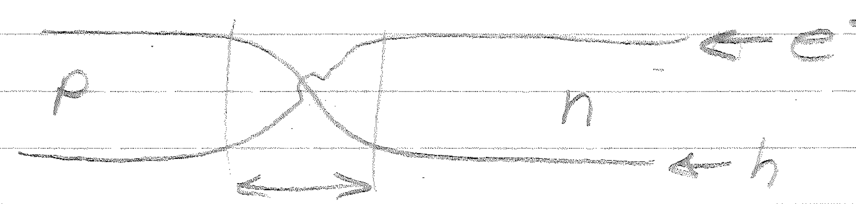
ALLOWS BOLTZMAN FACTOR USE

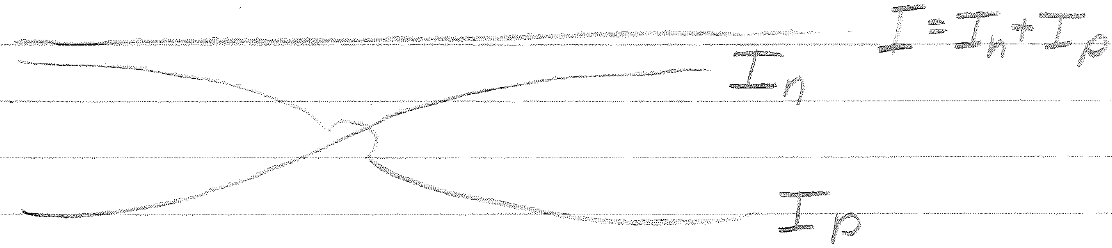
② BOLTZMAN APPROXIMATION

③ CONSTANT e & h CURRENT THRU DEPLETION LAYER (& THRU JUNCTION)

④ LOW LEVEL INJECTION

ELECTRON HOLE DENSITY





$V = V_a - V_j$

V_a = APPLIED BIAS VOLTAGE

V_j = BUILT IN JUNCTION BIAS

$n_p = n_n e^{(q/kT)(V_a - V_j)}$

$= n_{n_0} e^{qV_a/kT}$

E_c

$E = E_c - E_0$

E_0

IN COND. BAND = $N_D e^{-E/kT}$

$n_i^2 = np \Leftarrow$ MASS ACTION LAW

n_p = # OF e^- ON p SIDE WHEN V_a IS APPLIED

n_n = CONCENTRATION OF e^- ON n SIDE

$p_n = p_{n_0} e^{qV_a/kT}$

(I) CONTINUITY EQ: (OF CHARGE)

$$\frac{dn}{dt} = G - \frac{n - n_0}{\tau_n} + \frac{1}{q} \vec{\nabla} \cdot \vec{J_n}$$

G = RATE OF GENERATION OF e-h PAIRS

$n - n_0$ = EXCESS CARRIER DENSITY

HOLE CURRENT $\Rightarrow$ $\frac{dp}{dt} = G - \frac{p - p_0}{\tau_p} - \frac{1}{q} \vec{\nabla} \cdot \vec{J_p}$

II) CURRENT EQUATION
(FROM BOLTZMAN XPORT EQ.)

$$\vec{J}_n = q\mu_n n\vec{E} + qD_n \nabla n$$

$$\vec{J}_p = q\mu_p n\vec{E} - qD_n \nabla p$$

$$\mu = \frac{q}{m^*}\frac{\langle v^2\tau\rangle}{\langle v^2\rangle}$$

$$D = \frac{\langle v^2\tau\rangle}{3}$$

$$D_n = \frac{kT}{q}\mu_n$$

COMBINING I & II:
(IN 1-D)

III). $$D_n\frac{d^2n}{dx^2} + \mu_n\left[E\frac{dn}{dx} + \frac{n\,dE}{dx}\right] - \frac{n-n_0}{\tau_n} = 0$$

$$D_p\frac{d^2p}{dx^2} - \mu_p\left[E\frac{dp}{dx} + \frac{p\,dE}{dx}\right] - \frac{p-p_0}{\tau_p} = 0$$

NEGLECT $\frac{dE}{dx}$

ASSUME: $\frac{n-n_0}{\tau_n} = \frac{p-p_0}{\tau_p}$ ← CHARGE NEUTRALITY

IV) COMBINING, YOU GET: (ADDING)

$$D\frac{p\frac{d^2n}{dx^2} + n\frac{d^2p}{dx^2}}{p+n} + \mu E\frac{p\frac{dn}{dx} - n\frac{dp}{dx}}{p-n} - \frac{p-p_0}{\tau_p} = 0$$

μ = MODIFIED MOBILITY = $\frac{p-n}{\frac{n}{\mu_p} + \frac{p}{\mu_n}}$

$$D = \frac{n+p}{\frac{n}{D_p} + \frac{p}{D_n}}$$

USED BY EBER'S MOLL

LOW LEVEL INJECTION:

p/n ON n SIDE $\ll 1$

(CONTROLED BY MINORITY)

HIGH LEVEL INJ.

$p \simeq n$

REDUCES TO DIFFUSION Eq.
SINCE FIELD TERM BECOMES
NEGLIGIBLE.

FOR AN ABRUPT PN JUNCTION

$$J_p \text{ (ON } n \text{ SIDE)} = -qD_p \frac{dp}{dx}$$

ANSWER IS

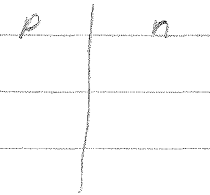
$$p - p_{no} = p_{no}\, e^{-x/L_p}\left(e^{\frac{qV_a}{kT}} - 1\right)$$

THIS IS FROM

$$\frac{d^2p}{dx^2} = \ldots$$

12-10-75 (WED)

REVIEW



"ABRUPT" ASSUMPTION

$n_p = n_{po} e^{qV_a/KT}$ = ELEC. ON P SIDE

$n_{po} = n_n e^{-qV_o/KT}$

I. CONSERVATION OF CHARGE

(ie CONTINUITY EQUATION)

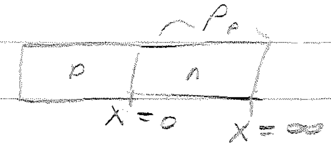
FOR ELECTRONS: $\frac{dn}{dt} = G - \underbrace{\frac{n-n_o}{\tau_n}}_{\text{DECAY}} + \frac{1}{q}\nabla \cdot J$

CURRENT DUE TO ELECTRONS

II. CURRENT: $J_n = \overbrace{q\underbrace{\mu}_{\text{MOBILITY}} n}^{\sigma} \vec{E} + qD_n \nabla n$

III FOR P-n JUNCTION

$J_p = -q_o D_p \frac{\delta p}{\delta x}$



$\frac{\delta p}{\delta x} \simeq \frac{\delta n}{\delta x}$

$$\left.\begin{aligned} P(x=0) &= P_{no} e^{qV_a/KT} \\ P(x=\infty) &= P_{no} \end{aligned}\right\} \text{BOUNDARY CONDITIONS}$$

IV. ASSUMING LOW LEVEL INJECTION:

$$\frac{\delta^2 p}{\delta x^2} - \frac{P - P_{no}}{D_p \tau_p} = 0$$

DEFINE: $L_p = \sqrt{D_p \tau_p}$

SOLN' IS $P - P_{no} = P_{no} e^{-x/L_p}\left[e^{\frac{qV_a}{KT}} - 1\right]$

$\Rightarrow J_p = \frac{q D_p P_{no}}{L_p}\left(e^{qV_a/KT} - 1\right)$

(L.L. INJECTION

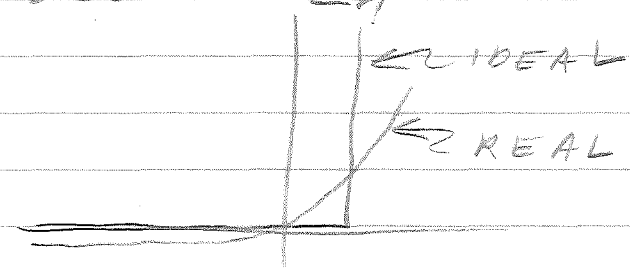
HOLE CURRENT DENSITY FOR A P-n JUNCTION

ELEC. CURRENT DENSITY FOR P-N JUNC:

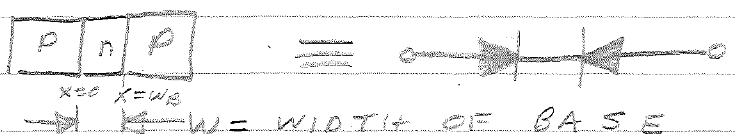
$$J_n = q n_{po} D_n / L_n \left(e^{qV_a/KT} - 1\right)$$

V). $J = J_{so}\left(e^{qV_a/KT} - 1\right)$

$$\Rightarrow J_{so} = \frac{q n_{po} D_n}{L_n} + q p_{no} D_p / L_p$$



ON TO PNP XSISTOR



EMITTER BIAS

$$p(x=0) = p_{no} e^{\frac{qV_E}{KT}}$$

USE AS B.C. FOR EQ IV GIVES

$$p(x) = p(x=0)\frac{\sinh\left(\frac{W_B - x}{L_p}\right)}{\sinh\left(W_B/L_p\right)}$$

$$J_p = -qD_p \frac{\partial p}{\partial x}$$

$$J_p\Big|_{\substack{EMITTER \\ x=0}} = q\,p(x=0)\frac{D_p}{L_p}\frac{\cosh(W_B/L_p)}{\sinh(W_B/L_p)}$$

$$J_p\Big|_{COLLECTER} = q\,p(x=0)\frac{D_p}{L_p}\frac{1}{\sinh(W_B/L_p)}$$

$$J_p\Big|_{EMIT} \sim J_p\Big|_{COL}$$

CRITICAL → $\Rightarrow \frac{W_B}{L_p}$ MUST BE A SMALL #

TOTAL CURRENT IN ϵ

$$\frac{I_\epsilon}{q} = (qD_n n_n/L_n)\left(e^{\frac{qV_\epsilon}{KT}} - 1\right) \leftarrow \text{EMITTER } e \text{ CURRENT}$$

$$+ \; qP_n(x=0)\underbrace{\frac{D_p}{L_p}}_{\epsilon \text{ HOLE CURRENT}} \frac{qV_\epsilon}{KT} \frac{\cosh w_B/L_p}{\sinh w_B/L_p}$$

TOTAL CURRENT IN C:

n_{pc} = EQUALIBRIUM VALUE OF n IN COLLECTOR (P TYPE)

$$\frac{I_c}{q} = \underbrace{\frac{qD_n n_{pc}}{L_n}}_{\text{ELECTRON COL CURRENT}} + qP_n(x=0)e^{qV_\epsilon/KT}\frac{D_p}{L_p}\frac{1}{\sinh\left(\frac{w_B}{L_p}\right)}$$

DEFINE $\alpha = \gamma \underline{\beta} \alpha^* = \frac{\delta I_c}{\delta I_\epsilon}$ (WANT $\alpha = 1$)

- $\gamma = \delta I_\epsilon(\text{HOLE}) / \delta I_\epsilon(\text{TOTAL})$

$$= \frac{1}{1 + \frac{D_n L_p n_{p1}}{D_p L_n P_{n2}} \frac{\cosh(w_B/L_p)}{\sinh(w_B/L_p)}}$$

= EMISSION EFFICIENCY OF FRACTION OF EMITTED CURRENT THAT IS HOLES.

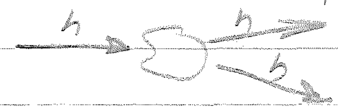
- $\underline{\beta} = \frac{dI_c(\text{HOLES})}{dI_\epsilon(\text{HOLES})}$

$$= \frac{1}{\cosh(w_B/L_p)}$$

= BASE TRANSPORT FACTOR (FRACTION OF EMITTED HOLES THAT MAKE IT TO THE COLLECTOR)

(ANOTHER $\beta \neq \underline{\beta}$; $\beta = \frac{I_c}{I_B}$)

$\alpha^* \equiv$ RATIO OF COLLECTOR CURRENT TO INCIDENT HOLE CURRENT.



ASSUME $\alpha^* \simeq 1$

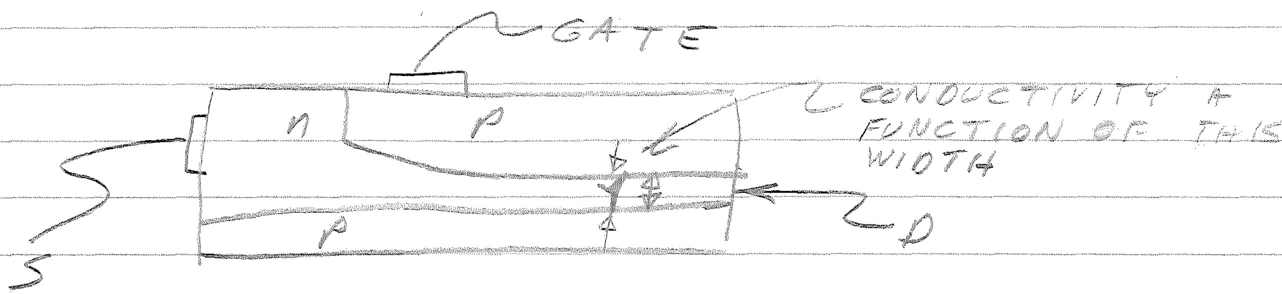
ACTUALLY: $\alpha^* = \frac{\sigma(\text{MINORITY})}{\sigma(\text{MAJORITY})} + 1$

σ = CONDUCTIVITY

MAKE $\gamma \simeq 1$: $P_p \Leftrightarrow N_A(E) > N_D(B)$

JUCTION FET

JFET $\Rightarrow$ WANT CONDUCTANCE



$dv = I_d \, dR$ $\qquad R \propto \frac{1}{\sigma}$

$dr = \frac{dx}{2YA\sigma_N}$ — CONDUCTIVITY

$$Y = \sqrt{\frac{2\epsilon}{q N_D}\left(V(x) + V_0 - V_{GS}\right)}$$

ASSUMING $N_D \ll N_A$

$\Rightarrow g_{DS} = \frac{\sigma a w}{L}$ $\quad \Rightarrow w$ = WIDTH WITH NO POTENTIAL

$$* \left[1 - \underbrace{\left(V_{DS} - V_{GS}\right)^{1/2}}_{\text{CONST}}\right]$$

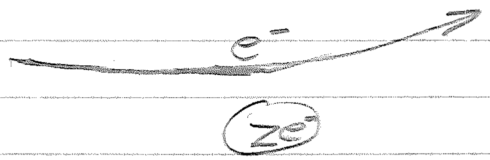
12-12-75 (FRI)

FINAL: 9 A.M. TUES.

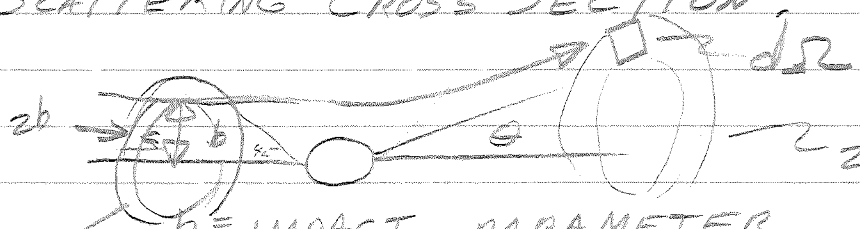
(HOW MANY e^- IN COND. BAND?)

- LITTLE TWO STATE
- NO HEAT DIFFUSION IN INSULATORS

IMPURITY SCATTERING IN SEMI-CONDUCTOR



SCATTERING CROSS SECTION:



$2\pi \sin\theta \, d\theta$

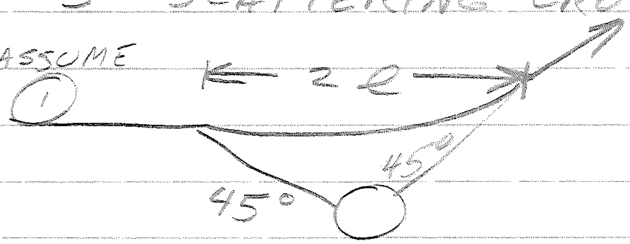
$b \equiv$ IMPACT PARAMETER

$A = 2\pi b \, db$

S = SCATTERING CROSS SECTION $= \dfrac{2\pi b \, db}{2\pi \sin\theta \, d\theta}$

ASSUME

(1)



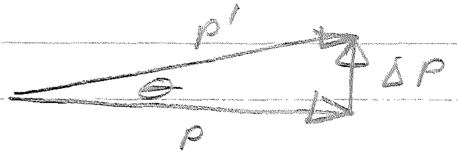
$F = \frac{dp}{dt} = \frac{Ze^2}{\epsilon \ell^2}$

(2) SCATTERING ANGLE SMALL

(3) ASSUME VELOCITY INITIAL $= V$

$\Delta t = \frac{2\ell}{v}$

THEN: $\Delta p = \frac{Ze^2 2}{bV}$



FOR SMALL ANGLE: $\frac{\Delta p}{p} = \theta$

$$\theta = \frac{\Delta p}{p} = \frac{Ze^2}{bmv^2}$$

ΔE = LOSS IN ENERGY

$$= (\Delta p)^2/2m$$

$$= 2Z^2e^4/mb^2v^2$$

REAL ANSWER IS

$$\tan\frac{\theta}{2} = \frac{Ze^2}{bmv^2}$$

GIVES

$$S = \left(\frac{Ze^2}{2Emv^2}\right)\frac{1}{\sin^4\left(\frac{\theta}{2}\right)}$$

IN A SOLID $\Rightarrow$ LET $mv^2 \propto kT$

TEST #1 (STUDY SHEET)

1 COMPTON EFFECT

1 THE BOHR ATOM

2 E AND V IN CM^{-1}

2 1-D SCHRÖ'S EQ'N

FREE PARTICLE SOLN'

INFINITE WELL SOLN

3 ENERGY LEVELS IN A SOLID

4 HARMONIC OSC

4 PHASE AND GROUP VELOCITIES

4 PAULI EXCLUSION PRINCIPLE

4 PERTURBED HARMONIC OSCILLATOR

5 BRILLOUIN ZONES

6 DISPERSION CURVES

6 BRILLOUIN ZONE FOR TWO MASSES

6 ATTENUATION (EVANASCENCE)

7 TRANSMISSION LINE EQUIVALENTS

8 DISPERSION CURVE IN 1D LATTICE

9 INTERPRETATION

10 A PERTURBATION

11 ELECTRONS IN A SOLID

12 IN THE OPTICAL MODE

12 MILLER INDICES

13 e^- HOLE INTERACTION

13 EFFECTIVE MASS

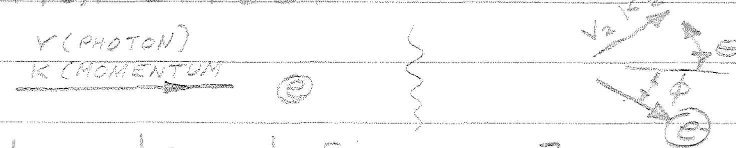
13 MEASURING EFFECTIVE MASS

14 ABSORPTION MEASUREMENT

I

I

- COMPTON EFFECT



$$\frac{1}{\omega_2} - \frac{1}{\omega_1} = \frac{1}{m}\left[1 - \cos\theta\right]$$

DESCRIPTION: A PHOTON HAVING ENERGY $E_1 = h\gamma_1$ "COLLIDES" WITH AN ELECTRON. PART OF THE ENERGY IS LOST TO THE NOW "MOVING" ELECTRON. THE PHOTON NOW HAS ENERGY $E_2 = \hbar\gamma_2 < E_1$. HERE, $\omega = 2\pi\gamma$.

- THE BOHR ATOM

BOHR MADE A MODEL OF THE HYDROGEN ATOM TO EXPLAIN OBSERVED QUATUM EFFECTS. HIS ASSUMPTIONS WERE

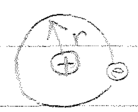
$E = K.E. + P.E = \frac{1}{2}mv^2 + \frac{Ze^2}{4\pi\epsilon r}$ ⇐ CONSERVATION OF ENERGY

$\frac{mv^2}{r} + \frac{Ze^2}{4\pi\epsilon r^2} = 0$ ⇐ Σ FORCES = 0

$L = n\hbar$ ⇐ ANGULAR MOMENTUM ASSUMP.

$E_2 - E_1 = h\gamma$ ⇐ QUANTIZED ENERGY ASSUMP.

THESE ASSUMPTIONS ARE FOR e^- CIRULAR ORBIT



e = ELECTRON CHARGE

$\hbar = \frac{\text{PLANCK'S CONSTANT} = h}{2\pi}$

Z = # ELECTRONS

PUTTING TOGETHER: $E_n = \frac{mZ^2e^4}{32\pi^2\epsilon^2 n^2\hbar^2}$ ⇐ ORBITAL ENERGIES

OR EQUIVALENTLY: $E_n - E_m = h\gamma_{nm} = \frac{mZ^2e^4}{32\pi^2\epsilon^2\hbar^2}\left(\frac{1}{n^2} - \frac{1}{m^2}\right)$

IONIZATION ENERGY IS GOTTON BY SETTING $m = \infty$, $n = 1 \Rightarrow E = R_H = \frac{mZ^2e^4}{32\pi^2\epsilon^2\hbar^2} = 13.6\,eV$

R_H IS THE RHYDBERG ENERGY OBSERVED EXPERIMENTALLY PRIOR TO BOHR'S MODEL.

- MEASURING E AND V IN cm^{-1}

  SINCE $E = h\nu = hc\frac{1}{\lambda}$, A PHOTON'S ENERGY OR FREQUENCY IS MANY TIMES GIVEN AS WAVELENGTH λ, IN INVERSE CENTIMETERS.

- SCHRÖDINGER'S EQUATION IN ONE DIMENSION

  $$-\frac{\hbar^2}{2m}\frac{\delta^2\psi}{\delta x^2} + (V-E)\psi = 0$$

  IT'S SOMETHING LIKE A CONSERVATION OF ENERGY: K.E. + P.E. = 0. ψ IS THE WAVE FUNCTION.

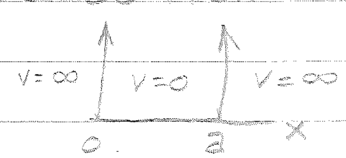
  I. SOLUTION FOR FREE PARTICLE ($V=0$)

  $$\frac{d^2\psi}{dx^2} + k^2\psi = 0 \quad \Rightarrow k^2 = \frac{-2mE}{\hbar}$$

  $$\Rightarrow \psi = Ae^{ikx} + Be^{-ikx} = \tilde{A}\sin kx + \tilde{B}\cos x$$

  $|\psi|^2$ IS A PROBABILITY DENSITY FUNCTION. FOR A FREE PARTICLE, WE DON'T KNOW AT ALL WHERE IT IS.

  II. SOLUTION IN AN INFINATE WELL



  BOUNDRY CONDITIONS DICTATE $\psi(a) = \psi(0) = 0$. APPLYING TO THE SOLUTION OF FREE PARTICLE, $B = 0$ AND $k = \frac{n\pi}{a}$.
  SINCE $k^2 = \frac{-2mE}{\hbar^2}$, WE HAVE

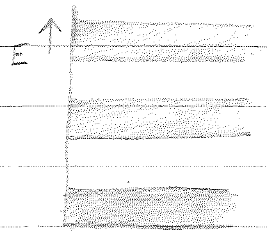
  $$E_n^2 = \hbar^2 n^2 \pi^2 / 2ma^2$$

  TO FIND A, USE THE FACT THAT

  $$\int_{-\infty}^{\infty}|\psi|^2 dx = A^2\int_0^a \sin^2 kx\, dx$$

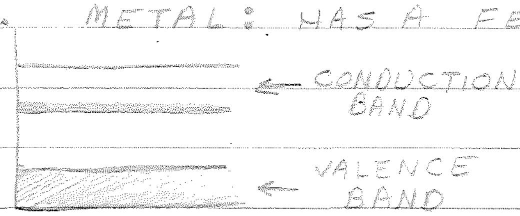
  GIVES $A = \sqrt{2/L}$ $\forall k$

ENERGY LEVELS IN A SOLID

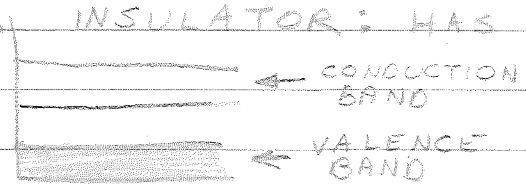


ALLOWED ENERGY STATES IN A SOLID

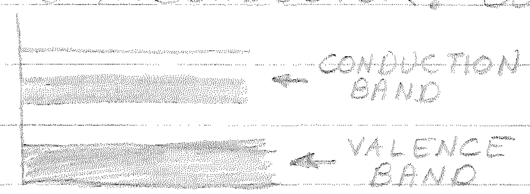
A. METAL: HAS A FEW ELECTRONS IN THE CONDUCTION BAND TO PLAY WITH



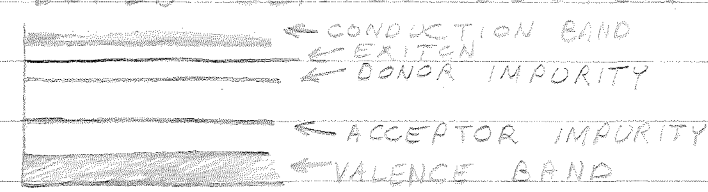
B. INSULATOR: HAS NO ELECTRONS IN THE CONDUCTION BAND.



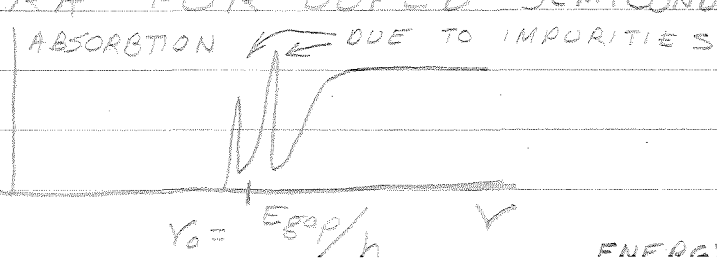
C. SEMICONDUCTOR: CONDUCTION BAND NOT FULL, NOT EMPTY



D. DOPED SEMICONDUCTOR



ANOTHER BAND OCCURS FROM AN EXITON (BOUND ELECTRON HOLE) PAIR. ABSORBTION SPECRA FOR DOPED SEMICONDUCTOR HAS BUMPS:



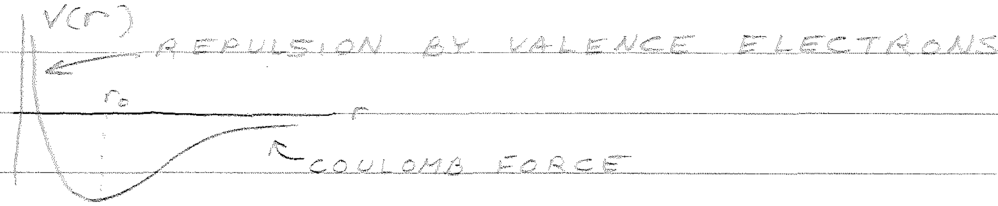
- SCHRÖ'S EQ: HARMONIC OSCILLATOR

$V = \frac{1}{2} m w^2 x^2$ ⇐ LIKE POTENTIAL OF A SPRING

IN ONE DIMENSION;

$$-\frac{\hbar^2}{2m}\frac{\delta^2}{\delta x^2}\psi + \frac{1}{2} m w^2 x^2 = E\psi$$

THE HARMONIC OSCILLATOR IS, FOR EXAMPLE, AN APPROXIMATION TO AN ATOM WHICH HAS A POTENTIAL SOMETHING LIKE:



A TAYLOR SERIES EXPANSION ABOUT r_0 WOULD GIVE, TO SECOND ORDER, A PARABOLA. ANYWAY, SOLUTION IN ONE DIMENSION GIVES "HERMITE POLYNOMIALS" AND EIGEN FREQUENCIES $E_n = (n + \frac{1}{2})\hbar\omega$

- VELOCITIES

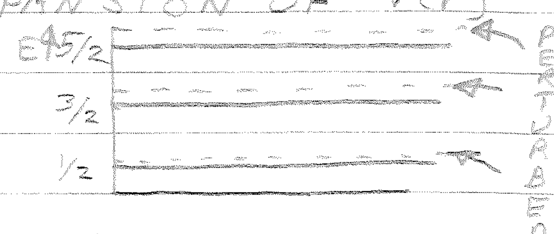
PHASE VELOCITY = $\frac{\omega}{k} = v\lambda$

GROUP VELOCITY = $\frac{d\omega}{dk}$

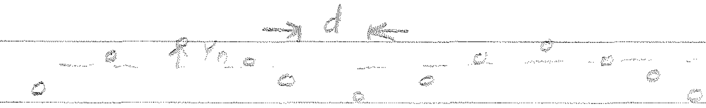
- PAULI EXCLUSION PRINCIPLE: NO TWO ELECTRONS CAN OCCUPY A STATE WITH THE SAME QUANTUM NUMBERS

- PERTURBED HARMONIC OSCILLATOR

$V = \frac{1}{2}\gamma x^2 + \text{cost}\, x^3$ $(\gamma = m w^2)$ IS A THIRD ORDER TAYLOR EXPANSION OF $V(r)$ ABOVE. EIGEN ENERGIES ARE SLIGHTLY INCREASED



BRILLOUIN ZONES

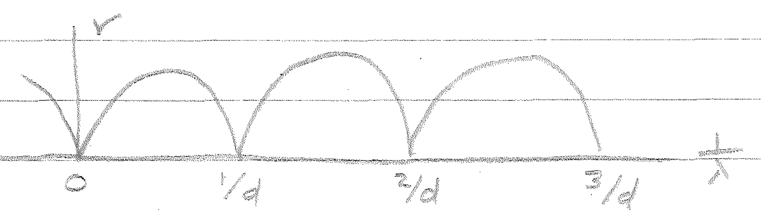


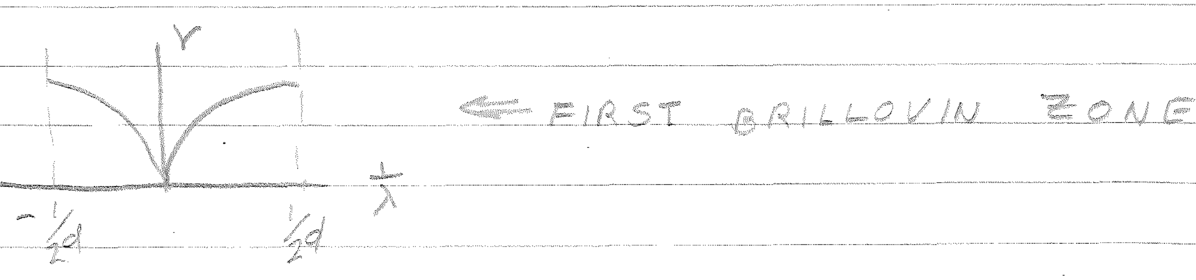
FOR WAVES IN A "ONE-DIMENSIONAL" SOLID, THE DISPLACEMENT OF AN ATOM, EITHER TRANSVERSE OR LONGITUDINAL, IS GIVEN BY

$$y_n = A \cos(\omega t - knd)$$

NOTE THAT SUBSTITUTION OF k BY $k + \frac{2\pi n}{d}$ WOULD GIVE THE SAME EXACT SOLUTION. THAT IS, THERE ARE A NUMBER OF SINUSOIDS THAT PASS THROUGH THE DISPLACEMENTS. THE FREQUENCY ν OF THE WAVE IS THUS PERIODIC WITH RESPECT TO THE WAVE NUMBER k. THE LOWEST ORDER OF THIS PERIODICITY IS TERMED THE BRILLOUIN ZONE.

$$\nu \propto \left|\sin \frac{\pi d}{\lambda}\right| = \left|\sin \frac{dk}{2}\right|$$



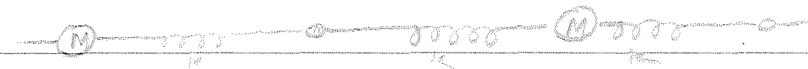


- DISPERSION CURVES

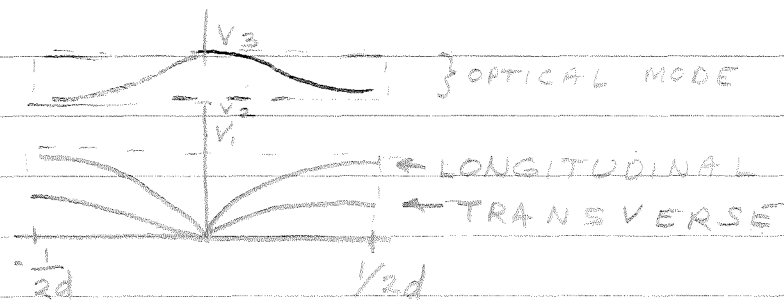
THE RELTIONSHIP BETWEEN ν AND $\frac{1}{\lambda}$, OR EQUIVALENTLY ω AND k, IS A DISPERSION CURVE. THE BRILLOUIN ZONE IS A DISPERSION CURVE.

- BRILLOUIN ZONE FOR UNEQUAL MASSES

MODELED AS:



PRODUCES A BRILLOUIN ZONE:



THE OPTICAL MODE VIBRATES LIKE THIS:

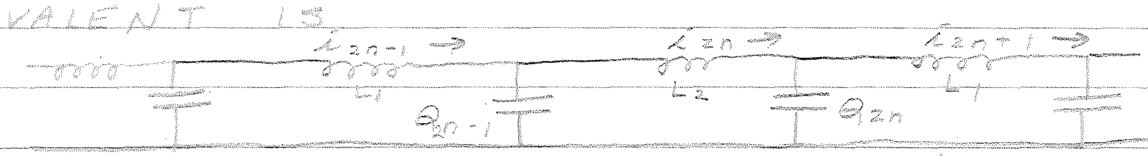
IT PRODUCES A DIPOLE MOMENT.

- ATTENUATION (EVANASCENCE)

IF A CRYSTAL IS EXCITED AT A FREQUENCY NOT ALLOWED FOR ON THE DISPERSION CURVE, IT IS ATTENUATED (OR IN THE EVANESCENT MODE)

TRANSMISSION LINE EQUIVALENTS

ONE DIMENSIONAL CRYSTALS ARE MATHEMATICALLY AKIN TO TRANSMISSION LINES. THAT IS, YOU GET DISPERSION CURVES FOR BOTH. FOR THE TWO MASS CASE, THE TRANSMISSION LINE EQUIVALENT IS



USING KIRCHOFF'S LAWS: $i_{2n} - i_{2n+1} = \frac{d}{dt} Q_{2n}$

$$i_{2n+1} - i_{2n+2} = \frac{d}{dt} Q_{2n+1}$$

ALSO $L_1 \frac{d i_{2n+1}}{dt} = \frac{i_{2n} - i_{2n+1}}{C_1} - \frac{i_{2n+1} - i_{2n}}{C_2}$

$$L_2 \frac{d i_{2n}}{dt} = \frac{i_{2n-1} - i_{2n}}{C_2} - \frac{i_{2n} - i_{2n+1}}{C_1}$$

USING $i_{2n} = A_2 e^{i(\omega t - 2nkx)}$

$$i_{2n+1} = A_1 e^{i(\omega t - (2n+1)kx)}$$

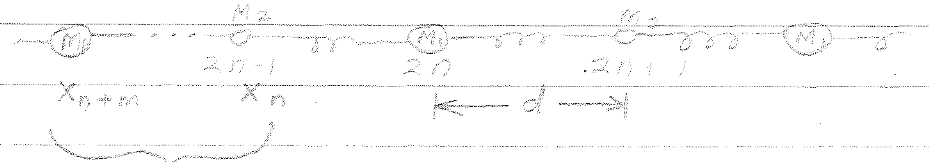
GIVES $\left[-L_1\omega^2 + \frac{1}{C_1} + \frac{1}{C_2}\right]A_1 - \left[\frac{e^{ikx}}{C_1} + \frac{e^{-ikx}}{C_2}\right]A_2 = 0$

$$\left[L_2\omega^2 + \frac{1}{C_1} + \frac{1}{C_2}\right]A_2 - \left[\frac{e^{-ikx}}{C_1} + \frac{e^{-ikx}}{C_1}\right]A_1 = 0$$

SETTING $\det|\;| = 0$ GIVES

$$\omega = \frac{1}{2}\left(\frac{1}{L_1} + \frac{1}{L_2}\right)\left(\frac{1}{C_1} + \frac{1}{C_2}\right) \pm \left[\frac{1}{4}\left(\frac{1}{L_1} + \frac{1}{L_2}\right)^2\left(\frac{1}{C_1} + \frac{1}{C_2}\right) - \frac{4\sin^2 kx}{L_1 L_2 C_1 C_2}\right]^{\frac{1}{2}}$$

DISPERSION CURVE FOR 1D LATTICE



$$U[|X_{n+m} - X_n|] = \text{POTENTIAL BETEEN } n \text{ AND } m^{TH} \text{ MASS}$$

$$= U(md) + (Y_{n+m} - Y_n)U'(md) + \frac{1}{2}(Y_{n+m} - Y_n)^2 U''(md) + \ldots$$

$$\simeq \sum_n \sum_{m>0} \Big[U(md) + (Y_{n+m} - Y_n)U'(md) + \frac{1}{2}(Y_{n+m} - Y_n)^2 U''(md) + \ldots \Big]$$

F_p = FORCE ON p^{TH} MASS

$$= -\frac{\delta U}{\delta Y_p} = -\frac{d}{dY} \sum_{m>0} (Y_{p+m} - Y_n)U'(md) + \frac{1}{2}(Y_{p+m} - Y_n)^2 U''(md) + \ldots$$

$$- \frac{d}{dY} \sum_{m>0} (Y_p - Y_{p-m})U'(md) + \frac{1}{2}(Y_p - Y_{p-m})^2 U''(md)$$

$$= \sum_{m>0} U''(Md) \left[Y_{p+m} + Y_{p-M} - 2Y_p \right]$$

IGNORING HIGHER ORDERED TERMS:

$$F_{2n} = U_1''(Y_{2n-1} + Y_{2n+1} - 2Y_{2n}) = M_2 \frac{d^2 Y_{2n}}{dt^2}$$

$$F_{2n+1} = U_2''(Y_{2n} + Y_{2n+2} - 2Y_{2n+1}) = M_1 \frac{d^2 Y_{2n+1}}{dt^2}$$

ASSUME SOLUTIONS:

$$Y_{2n} = A_2 e^{i(\omega t - nkd)} \; ; \; Y_{2n+1} = A_1 e^{i(\omega t - \frac{2n+1}{2}kd)}$$

GIVES:

$$A_2(M_2\omega^2 - 2U_1'') + 2A_1 U_1'' \cos\frac{kd}{2} = 0$$

$$A_1(M_1\omega^2 - 2U'') + 2A_2 U_1'' \cos\frac{kd}{2} = 0$$

$\det|\;| = 0$ GIVES

$$\omega^2 = U_1''\left[\left(\frac{1}{M_1} + \frac{1}{M_2}\right) \pm \sqrt{\left(\frac{1}{M_1} + \frac{1}{M_2}\right)^2 - \frac{4\sin^2 kd}{M_1 M_2}}\right]$$

INTEPRETATION OF 1-D LATTICE DISPERSION CURVE

THE DISPERSION CURVE RELATIONSHIP MAY BE REWRITTEN AS:

$$\omega^2 = \frac{U_1''}{M_1 M_2}\left[M_1 + M_2 \pm \sqrt{M_1^2 + M_2^2 + 2M_1M_2 \cos kd}\right]$$

WLOG, ASSUME THAT $M_1 > M_2$

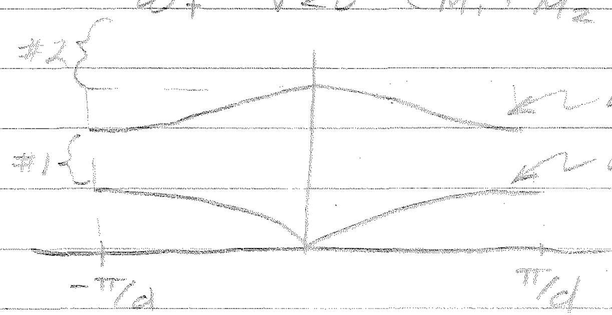
FOR LONG WAVELENGTHS, $\lambda >> d$ AND $k << \frac{1}{d}$

$$\Rightarrow \cos kd \simeq 1 - \frac{k^2 d^2}{2}$$

$$\Rightarrow \sqrt{M_1^2 + M_2^2 + 2M_1M_2 \cos kd} \simeq M_1 M_2 \left[1 - \frac{k^2 d^2 M_1 M_2}{2(M_1 + M_2)}\right]$$

$$\omega_- = kd\sqrt{\frac{U_1''}{2(M_1 + M_2)}}$$

$$\omega_+ = \sqrt{2U''\left(\frac{1}{M_1} + \frac{1}{M_2}\right) - \frac{k^2 d^2}{4(M_1 + M_2)}}$$



AT THE FORBIDDEN ZONES

$\sin kd/2 > 1$

$$kd = \alpha + i\beta$$

$$\sin {kd}/{2} = \sin\frac{\alpha}{2}\cosh\frac{\beta}{2} + i\cos\frac{\alpha}{2}\sinh\frac{\beta}{2}$$

$$\alpha = 0, \Rightarrow k = {i\beta}/{d}$$

I

A PERTURBATION

SCHRODINGERS EQ'N IS:

$$i\hbar \frac{\delta \psi}{\delta t} = H\psi = E_n \psi$$

ADD A PERTURBATION V:

$$i\hbar \frac{d\psi}{\delta t} = (H+V)\psi = (E_n + E_n^*)\psi$$

WITHOUT PERTURBATION:

$$\psi = \sum_n a_n \varphi_n(x)\, e^{-iE_n t/\hbar}$$

ASSUME, WITH PERTURBATION, $a_n = a_n(t, x)$

PLUG INTO PERTURBED EQ. RECOGNIZING ORTHONALITY OF ψ_n, THIS GIVES

$$\frac{\delta a_s}{\delta t} = \frac{-i}{\hbar} \sum_n a_n V_{sn}\, e^{i/\hbar (E_s - E_n)t}$$

$V_{sn} = \int \phi_s^* V \phi_n \, dx \Leftarrow$ MATRIX ELEMENT

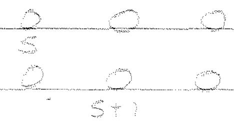
RECALL $\int \phi_s^* H \phi_n \, dx = E_n \delta_{ns}$.

THE MATRIX ELEMENT, V_{sn}, IS A COUPLING TYPE NUMBER, AND CAN BE MEASURED EXPERIMENTALLY.

FOR THE SPECIAL CASE WHERE $E_s = E_n$,

$$\frac{\delta a_s}{\delta t} = \frac{-i}{\hbar} \sum_n a_n V_{sn}$$

● ELECTRONS IN A SOLID



ASSUME $a = e^{-i\omega t}$

$$\hbar\omega a_s = E a_s = \sum_n a_n V_{sn}$$

$$E_0 = V_{ss} \Rightarrow E a_s = E_0 a_s + V_{s,s+1} a_{s+1} + V_{s,s-1} a_{s-1} - -$$

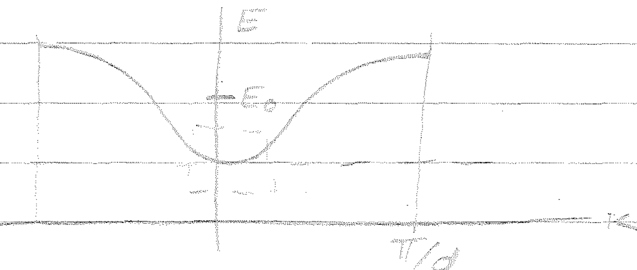
ASSUME e JUMP ONLY TO ADJACENT ATOMS:

$$E a_s \simeq E_0 a_s - V_{s,s+1} a_{s+1} - V_{s,s-1} a_{s-1}$$

$$(E - E_0) a_s = -V(a_{s-1} + a_{s+1})$$

LET $a_{s+n} = e^{iknd}$, $a_{s-n} = e^{-iknd}$

$$\Rightarrow E = E_0 - 2V_1 \cos kd$$



AT K NEAR 0, $\cos kd = 1 - \frac{k^2}{2d^2}$

$$\Rightarrow E = E_0 - 2V_1 + V_1 d^2 k^2 \Leftarrow$$ PAROBOLA (HARMON. OSC)

RECALL THAT FOR AN ELECTRON IN FREE SPACE:

$E = \frac{\hbar^2 k^2}{2m} \Rightarrow m =$ EFFECTIVE MASS $= \frac{\hbar^2}{2V_1 d^2}$

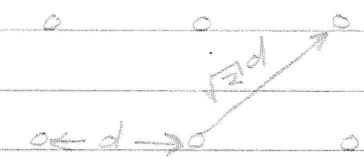
- ELECTRONS IN A SOLID: OPTICAL MODE

THE LAST EFFORT WAS AN APPROXIMATION

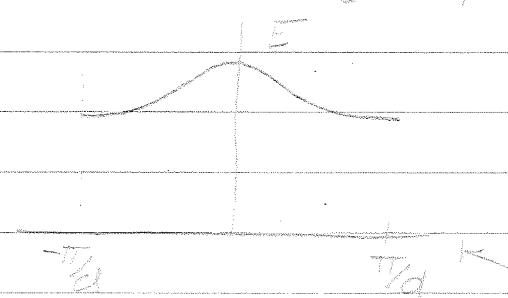
TO $i\hbar \frac{\delta a_s}{\delta t} = E_0 a_s + \sum_n V_{s+n}\, a_{s+n}$

IF YOU ASSUME ELECTRONS

CAN JUMP DIAGONALLY



YOU GET $E = E_0 - 2V_1 \cos kd - 2V_2 \cos k\sqrt{2}d$



- MILLER INDICES

TO SPECIFY DIRECTIONS IN A

CRYSTAL, YOU USE MILLER INDICES.

IF YOU GO a IN THE X DIRECTION,

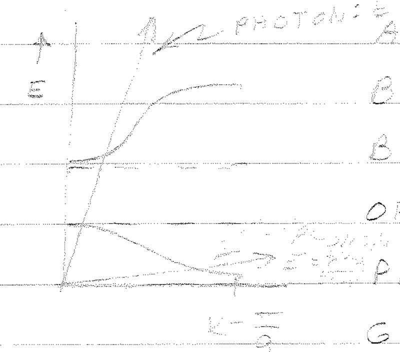
b IN THE Y, AND c IN THE Z,

AND THE CRYSTAL STARTS ITS

PERIOD OVER, THEN THE

MILLER INDICE IS $\left(\frac{1}{a}, \frac{1}{b}, \frac{1}{c}\right)$

ELECTRON-HOLE INTERACTION



AN ELECTRON IN THE CONDUCTION BAND AND A HOLE IN THE VALENCE BAND MAY COMBINE TO GIVE OFF A PHOTON WITH ENERGY PROPORTIONAL TO THE ENERGY GAP PLUS AN EXTRA PHONON:

$$e_{CB} + h_{VB} \longrightarrow (e,h)_{VB} + h\nu_{(E_{CB} - E_{VB})}$$

MOMENTUM MUST BE CONSERVED

THUS: $\vec{k}_e + \vec{k}_h \rightarrow \sim 0 + \vec{k}_p$

EFFECTIVE MASS

$V_g = \frac{d\omega}{dk}$ $\quad \frac{dV_g}{dt} = F/m^* \Rightarrow m^* = \text{EFFECTIVE MASS}$

USING $E = \hbar\omega \Rightarrow V_g = \frac{1}{\hbar}\frac{\partial E}{\partial k}$

$$\Rightarrow \frac{dV_g}{dt} = \frac{\partial V_g}{\partial k}\frac{\partial k}{\partial t} = \frac{1}{\hbar}\frac{\partial^2 E}{\partial k^2}\frac{\partial k}{\partial t} \Rightarrow m^* = \frac{\hbar^2}{\partial^2 E/\partial k^2}$$

MEASURING EFFECTIVE MASS

PUT A MAGNETIC FIELD $\vec{B}_z$ ON A PARTICLE OF q

$$\left.\begin{aligned} F_y &= qV_xB = m_y^*\ddot{y} \\ F_x &= -qV_yB = m_x^*\ddot{x} \end{aligned}\right\} \text{WILL GIVE ELLIPTICAL PATH}$$

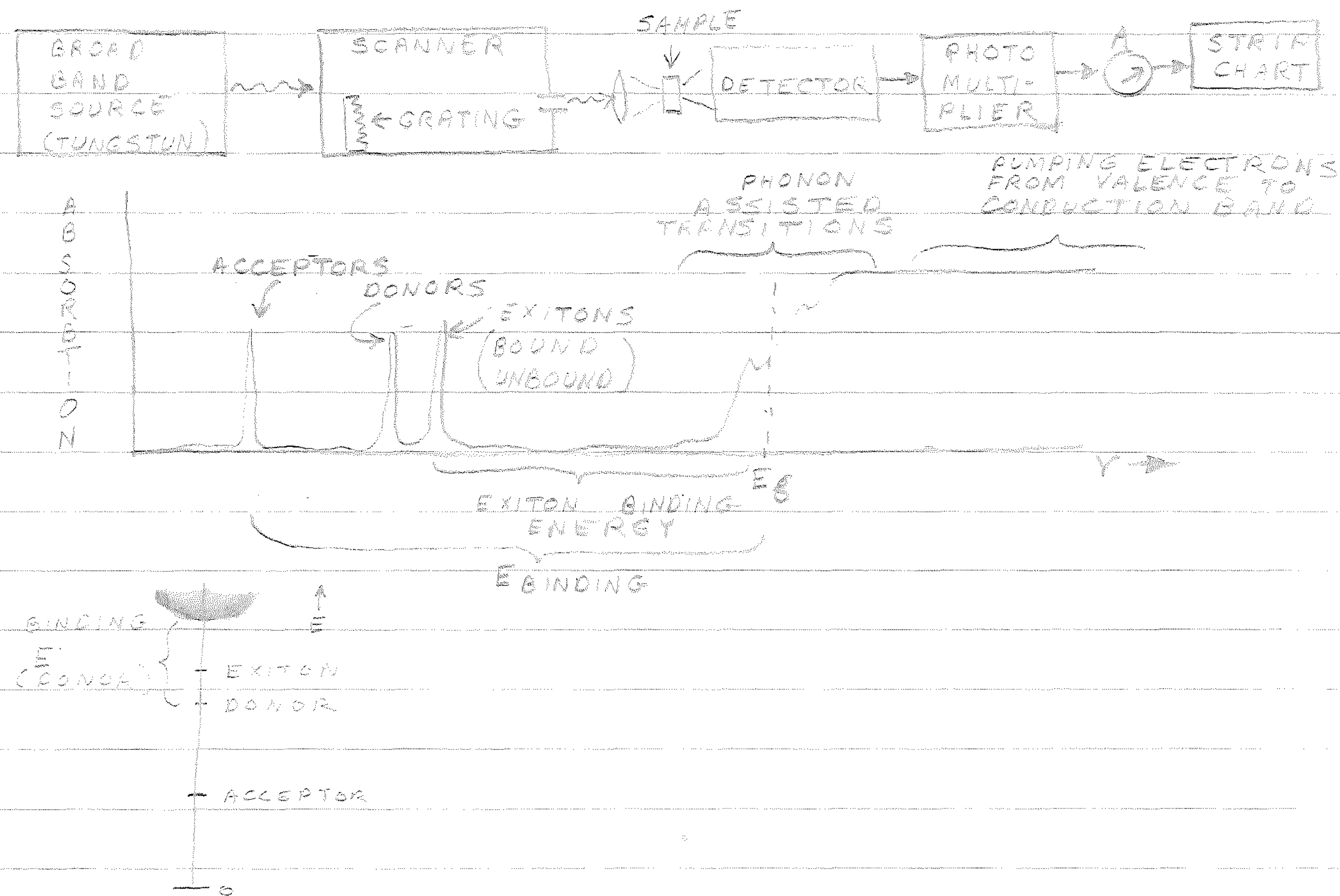
ASSUMING $m = m_x^* = m_y^*$ (NOT ALWAYS TRUE)

$$m(\ddot{x} + \ddot{y}) = qB(\dot{x} - \dot{y})$$

ASSUMING $x = A\sin\omega_0 t$, $y = A\cos\omega_0 t$

GIVES $\omega_0^2 = (qB/m^*)^2$

ABSORBTION MEASUREMENT



TO FIND THE ABSORBTION SPECTRA AT LOW T, SAMPLE IS PLACED IN A "DEWAR"

- THE FERMI-DIRAC DISTRIBUTION DEFINITION

n = # ELECTRONS IN CONDUCTION BAND

p = # HOLES IN VALENCE BAND

$$n(E) = f(E)\,e(E) \Rightarrow f(E) = n(E)/e(E)$$

$f(E)$ = FERMI-DIRAC DISTRIBUTION

$= P[e^- \text{ HAS ENERGY } E]$

$e(E)$ = # OF QUANTUM STATES AS A FUNC. OF E

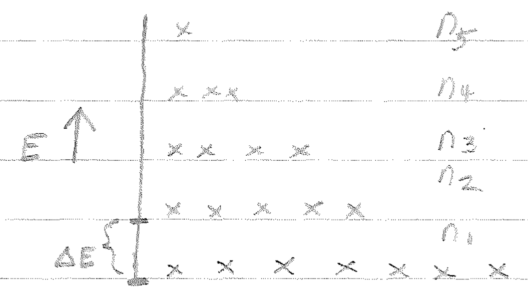
$n(E)$ = # OF ELECTRONS WITH ENERGY E

$$n = \int n(E)\,dE = \int f(E)\,e(E)\,dE$$

ASSUMPTIONS: 1. THERMAL EQUALIBRIUM

2. PAULI'S EXCLUSION PRINCIPLE

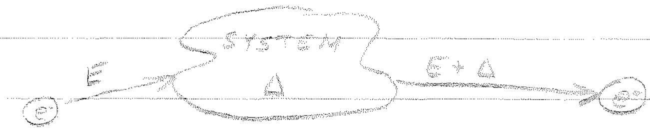
- BOLTZMAN FACTOR



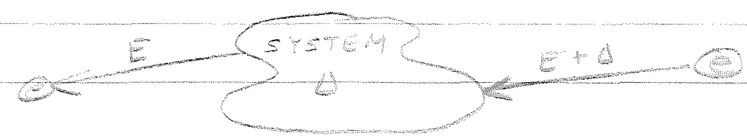
n_i = NUMBER OF e^-'S WITH ENERGY E_i

$$\frac{n_2}{n_1} \cong e^{-\Delta E/KT} = \text{BOLTZMAN FACTOR}$$

- FERMI-DIRAC DISTRIBUTION DERIVATION



$P[\text{OUTPUT}] = f(E)\, P[E \rightarrow E+\Delta E]\,[1 - f(E+\Delta)]$



$P[\text{OUTPUT}] = f(E+\Delta)\, P[E+\Delta E \rightarrow E]\,[1 - f(E)]$

EQUATING GIVES

$$\frac{P[E \rightarrow E+\Delta E]}{P[E+\Delta \rightarrow E]} = \frac{f(E+\Delta)}{f(E)} \frac{[1 - f(E)]}{[1 - f(E+\Delta)]}$$

$$= e^{-\Delta E/kT} = \text{BOLTZMAN FACTOR}$$

SOLVING FOR $f(E)$ GIVES

$$f(E) = \frac{1}{e^{(E-E_F)/kT} + 1}$$

- $n(E)$ = # ELECTRONS WITH ENERGY E

$= P[e^- \text{ CAN HAVE ENERGY } E]\, dn$

dn = NUMBER OF BOXES TO PUT E INTO

$$n(E) = f(E)\, dn$$

RECALL THAT FOR AN INFINATE WELL

$$E_n = n^2 \left(\frac{\hbar^2 \pi^2}{2mL^2}\right) \Rightarrow n = \frac{\sqrt{2m}\, L}{\hbar \pi} \sqrt{E}$$

THEREFORE: $dn = \frac{1}{2}\left(\frac{2mL^2}{\hbar^2 \pi^2}\right)^{\frac{1}{2}} \frac{1}{\sqrt{E}}$ ⟸ ONE DIMENSION

FOR THREE DIMENSIONS, $dn^{(3)} = \frac{1}{8}(4\pi n^2 dn)$. (SURFACE AREA OF A SPHERE). THE $\frac{1}{8}$ IS PUT IN TO SINGLE OUT THE FIRST OCTANT. ANY WAY, THIS GIVES

$$dn^{(3)} = (\quad)\sqrt{E}\, dE \ni (\quad) \text{ IS CONSTANT}$$

$$n(E) = f(E)\, dn^{(3)} = \text{CONST} \sqrt{E} \left(\frac{1}{e^{\frac{E-E_F}{kT}} + 1}\right)$$

I

- EFFECTIVE DENSITY OF STATES

$n = \int_{E_c}^{\text{TOP OF BAND}=\infty} n(E)\,dE$ = ELECTRONS IN COND. BAND

$= \text{CONST} \int_{E_c}^{\infty} \frac{\sqrt{E-E_c}}{1+e^{(E-E_F)/kT}}\,dE$

$\cong \text{CONT} \int_{E_c}^{\infty} \sqrt{E-E_c}\; e^{-(E-E_F)/kT}\,dE$

THIS APPROXIMATION IS GOOD AT ROOM TEMPERATURE SINCE kT IS SO SMALL.

$(\therefore e^{(E-E_F)/kT} >> 1)$

$n \cong 2\left(\frac{2\pi m_e kT}{h^2}\right) e^{-(E_c-E_F)/kT}$

$= N_c\, e^{-(E_c-E_F)/kT}$ = EFFECTIVE DENSITIES OF STATE

p = # HOLES IN VALENCE BAND

$= 2\left(\frac{2\pi m_h kT}{h^2}\right) e^{-(E_c-E_F)/kT}$

$= N_v\, e^{-(E_F-E_c)/kT}$

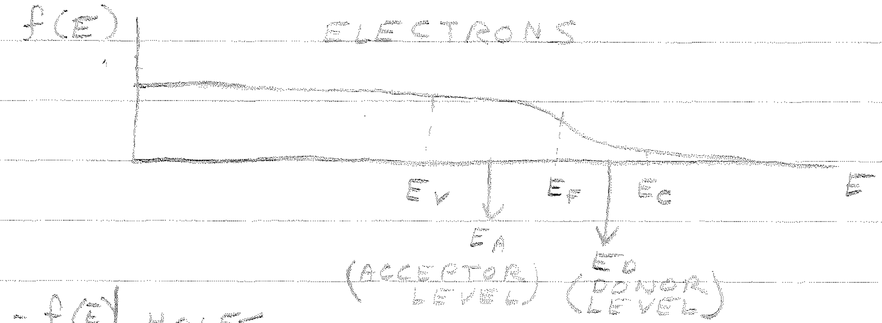
- MASS-ACTION LAW

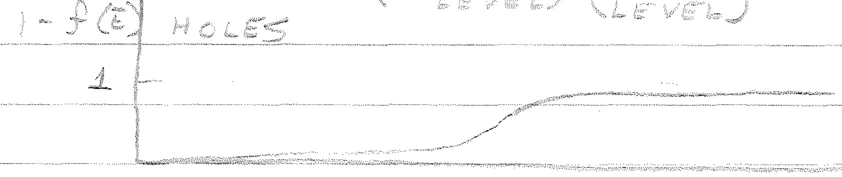
$np = N_c N_v\, e^{-(E_c-E_v)/kT}$

$= N_c N_v\, e^{-E_g/kT}$

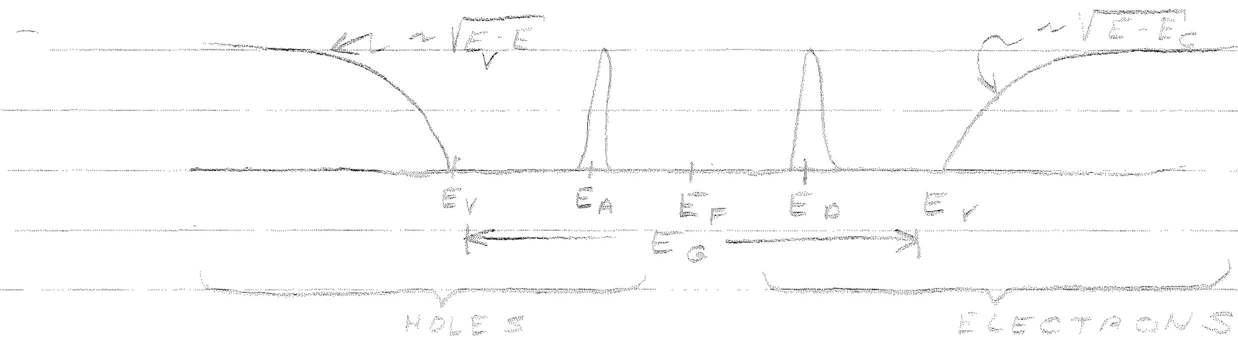
E_g = ENERGY GAP $= E_c - E_v$

• FERMI-DISTRIBUTION GRAPHS

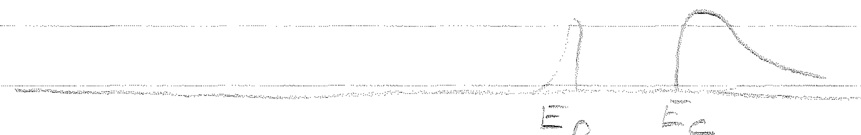




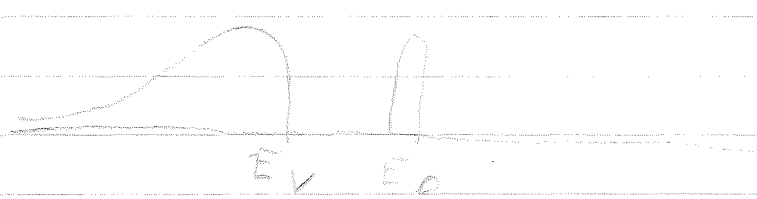
• DENSITY OF STATE GRAPHS



FOR HOLES: $n(E) = [1 - f(E)]\rho(E)$



FOR ELECTRONS: $n(E) = \rho(E)\, f(E)$



IMPURITY DISTRIBUTION FUNCTION

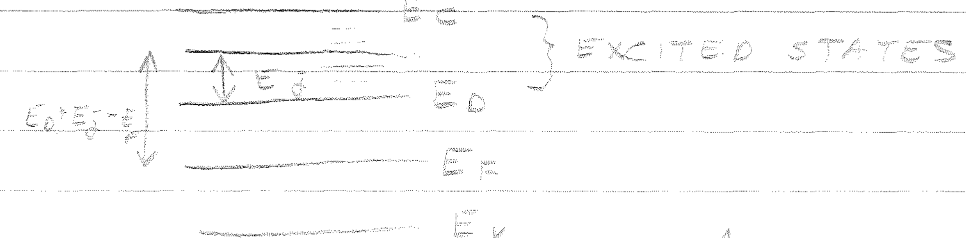
FOR DONORS

ASSUME 1 ELEC. ON DONOR

f_j = IMPURITY DISTRIBUTION FUNCTION

= P[e^- IS IN STATE j IN DONOR COMPLEX]

= P[NO e^- IS ON DONOR] P[e^- HAS ENERGY E_j]



$$f_j = \left[1 + \sum_{i \neq j} f_i\right] \cdot \frac{1}{1 + e^{(E_D + E_j - E_F)/kT}}$$

F^+ = P[DONOR HAS NO ELECTRON]

$$f_i = F^+ e^{-\mathcal{J}} \ni \mathcal{J} = (E_D - E_j - E_F)/kT$$

GIVES $F^+ = \left[1 + \sum_j e^{\mathcal{J}}\right]^{-1} = n_D/N_D$

n_D = # e^- IN COND. BAND FROM DONORS

N_D = # DONOR ATOMS

ALLOWING FOR DEGENERACY

$$F^+ \cong \frac{}{1 + g_G e^{-\mathcal{J}_{GRD}}} = \frac{1}{1 + g e^{-(E_D - E_F)}}$$

$\mathcal{J}_{GRD} = E_D - E_F$

g_G = DEGENERACY OF GROUND STATE

EFFECTS OF DOPING ON FERMI LEVEL

$n = \#\ e^-$ IN CONDUCTION BAND FROM DONORS

$= N_c e^{-(E_c - E_F)/kT}$

N_D = NUMBER OF DONORS

N_D^0 = NUMBER OF NEUTRAL DONORS

$n \cong N_D - N_D^0$

AT HIGH TEMP: $E_F = E_c - kT \ln \frac{N_c}{N_D}$

AT LOW TEMP: $E_F = \frac{E_c + E_D}{2} + \frac{kT}{2} \ln \frac{N_c g}{N_D}$

g = DEGENERACY

TEST #2 (STUDY SHEET)

1. SPECIFIC HEAT (HARMONIC OSCILLATOR)
2 DEBYE'S MODEL
3 ELECTRON CONTRIBUTION TO SPECIFIC HEAT
4 HARMONIC OSCILLATOR (RIGOROUS SOLN.)
5 MATRIX ELEMENTS
5 FERMI'S GOLDEN RULE
6 RUTHERFORD SCATTERING
7 HEAT DIFFUSION (RADIAL)
8 " " (TRANSVERSE)
9 TWO STATE QUANTUM SYSTEM
10 BOLTZMAN TRANSPORT EQUATION

II

- SPECIFIC HEAT
  - $C_V = \left.\frac{\delta E}{\delta T}\right|_V$

    CLASSICALLY, IN A GAS, $E = 3NkT \Rightarrow C_V = 3Nk$
  - FOR A HARMONIC OSCILLATOR

    $E_n = (n+\frac{1}{2})\hbar\omega$ ⇐ SOLN. OF SCHRÖ'S EQN.

    $N_{n+1}/N_n = e^{-(E_{n+1}-E_n)/kT}$ ⇐ BOLTZMAN FACTOR

    $= e^{-\hbar\omega/kT}$ ⇐ FOR HARMONIC OSCILLATOR

    $\langle n \rangle$ = AVE # OF QUANTA IN A STATE n

    $= \sum_{n=0}^{\infty} n e^{-n\hbar\omega/kT} \Big/ \sum_{n=0}^{\infty} e^{-n\hbar\omega/kT}$

    $= -\frac{d}{d(\hbar\omega/kT)} \sum_{n=0}^{\infty} e^{-n\hbar\omega/kT} \Big/ \sum_{n=0}^{\infty} e^{-n\hbar\omega/kT}$

    $\sum_{n=0}^{\infty} e^{-n\hbar\omega/kT} = \frac{1}{1-e^{-\hbar\omega/kT}}$ ⇐ FROM Σ OF GEOMETRIC SERIES

    GIVES $\langle n \rangle = \frac{1}{e^{+\hbar\omega/kT}-1}$ ⇐ FOR BOSONS

    (FERMION'S OBEY PAULI EXCLUSION PRINCIPLE, BOSONS DON'T. FOR FERMIONS, FROM THE FERMI-DIRAC DISTRIBUTION, $\langle n \rangle = \frac{1}{e^{(E-E_F)/kT}+1}$)

    NOTE, FOR SMALL T, $\langle n \rangle \cong kT/\hbar\omega$

    $\langle E \rangle = \langle n \rangle \hbar\omega = kT$ ⇐ CLASSICAL RESULT

    GENERALLY: $\langle E(\omega) \rangle = \frac{N\hbar\omega}{e^{\hbar\omega/kT}-1}$

    $$\Rightarrow C_V = \left.\frac{\delta\langle E\rangle}{\delta T}\right|_V = Nk\left(\frac{\hbar\omega}{kT}\right)^2 \frac{e^{\hbar\omega/kT}}{(e^{\hbar\omega/kT}-1)^2}$$

II SPECIFIC HT (HAR. OSC. DEFN)

- DEBYE'S MODEL

$\langle E \rangle = \hbar\omega \langle n \rangle \Rightarrow E_{TOTAL} = \int \hbar\omega \langle n \rangle \left(\frac{dn}{dE}\right) dE$

$\frac{\delta n}{\delta E}$ = DENSITY OF STATES

DEBYE ASSUMED

① $\frac{dn}{dE} = \frac{\mathbb{V}\omega^2}{2\pi^2\hbar V^3}$, V = VELOCITY, $\mathbb{V}$ = VOLUME

② $\omega = Vk \Leftarrow$ LINEAR DISPERSION CURVE;

③ ω_D = MAXIMUM FREQUENCY = DEBYE FREQUENCY

$$E = \int_0^{\omega_D} \frac{\mathbb{V}\omega^2}{2\pi^2 V^3} \left(\frac{\hbar\omega}{e^{\hbar\omega/kT}-1}\right) d\omega$$

$$= \frac{3\mathbb{V} k^4 T^4}{2\pi^2 V^3 \hbar^3} \int_0^{\Theta_D/T} \frac{x^3\,dx}{e^x - 1}$$

Θ_D = DEBYE TEMPERATURE $= \frac{\hbar\omega_D}{k}$

$$C_V = 9Nk\left(\frac{T}{\Theta_D}\right)^3 \int_0^{\Theta_D/T} \frac{x^4 e^x\,dx}{(e^x-1)^2}$$

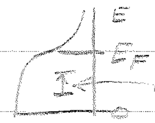
$$\cong \frac{12}{5}\pi^4 Nk \left(T/\Theta_D\right)^3 \text{ FOR SMALL } T$$

II DEBYE'S MODEL

ELECTRON CONTRIBUTION TO SPECIFIC HEAT

CLASSICALLY: $E = \frac{3}{2} kTN \Rightarrow C_V = \frac{3}{2} kT$

THIS DON'T WORK OUT TO WELL DUE TO PAULI'S EXCLUSION PRINCIPLE:



← FERMI-DIRAC DISTRIBUTION

INVALID TRANSITION DUE TO PAULI EXCLUSION PRINCIPLE

RECALL $E_F = \frac{\hbar^2}{2m}(3\pi^2 n)^{2/3}$

$$\frac{dn}{dE} = \frac{V}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\sqrt{E}$$

$$\Delta E = \text{ALLOWED E STATES} = \int_{E_F}^{\infty} E\, P_{FD}(E)\, \frac{dn}{dE}\, dE$$

$$= \frac{1}{4}\pi^2 N k\, T^2/T_F$$

WHERE $T_F = E_F/k$

$$\Rightarrow C_V = \frac{d\Delta E}{dT} = \frac{\pi^2}{2} N k\, T/T_F$$

II C_V (ELECTRON CONTRIBUTION)

● RIGOUROUS SOLUTION TO SIMPLE HARMONIC OSC.

$$-\frac{\hbar^2}{2m}\frac{\delta^2\psi}{\delta x^2} + (E-V)\psi = 0 \Leftarrow \text{1-D SCHRÖ'S EQN}$$

$$V(x) = \tfrac{1}{2}m\omega^2 x^2 \Leftarrow \text{HARMONIC OSCILLATOR POTENTIAL}$$

LET $\xi = \sqrt{\frac{m\omega}{\hbar}}\,x$; $\mathcal{E} = {}^{2E}/_{\hbar\omega}$

GIVES: $\frac{\delta^2\psi}{\delta\xi^2} + (\mathcal{E} - \xi^2)\psi = 0$

SUBSTITUTING $\psi = v e^{-\xi^2/2}$ GIVES HERMITE'S DIFF. EQN:

$$\frac{\delta^2 v}{\delta\xi^2} - 2\xi\frac{\delta v}{\delta\xi} + (\mathcal{E}-1)v = 0$$

IN ORDER FOR THINGS NOT TO BLOW UP, IT TURNS OUT

$$E = (n+\tfrac{1}{2})\hbar\omega$$

SOLN' IS THEN HERMITE POLYNOMIALS:

$$v = H_n(\xi) = (-1)^n e^{\xi^2}\frac{d^n}{d\xi^n}e^{-\xi^2}$$

THE WAVE FUNCTION IS: $\psi_n = H_n e^{-\xi^2/2}$

● HERMITE POLYNOMIALS AND WAVE FUNCTION

$$H_n(\xi) = (-1)^n e^{\xi^2}\frac{d^n}{\delta\xi^n}e^{-\xi^2} \Leftarrow \text{GENERATING FUNCTION}$$

$H_0(\xi) = 1$ $\qquad$ $H_2(\xi) = 4\xi^2 - 2$

$H_1(\xi) = 2\xi$ $\qquad$ $H_3(\xi) = 8\xi^3 - 12\xi$

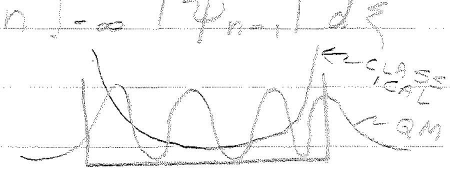
$$\frac{dH_n(\xi)}{\delta\xi} = 2n H_{n-1}(\xi)$$

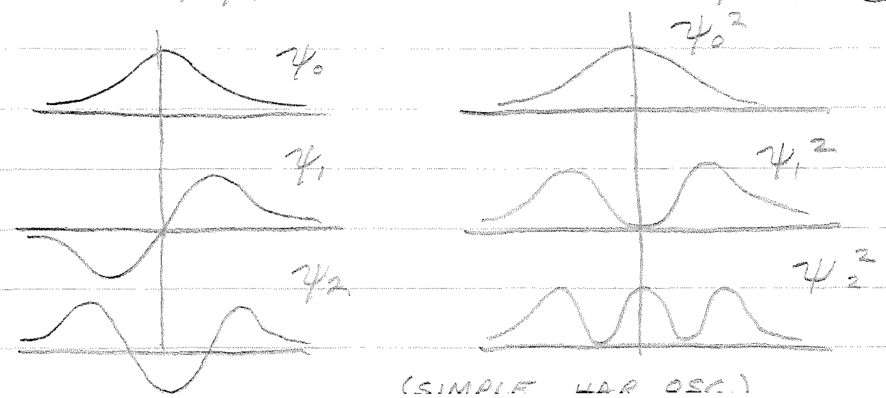
$$\psi_n = H_n e^{-\xi^2/2}$$

$$\int_{-\infty}^{\infty} H_n^2 e^{-\xi^2} d\xi = \int_{-\infty}^{\infty} |\psi_n|^2 d\xi = \sqrt{\pi}\, 2^n n!$$

$$= 2n\int_{-\infty}^{\infty} H_{n-1}^2 e^{-\xi^2} d\xi = 2n\int_{-\infty}^{\infty} |\psi_{n-1}|^2 d\xi$$

$$\begin{cases} \xi\psi_n + \dfrac{\delta\psi_n}{\delta\xi} = \sqrt{2n}\,\psi_{n-1} \\ \xi\psi_n - \dfrac{\delta\psi_n}{\delta x} = \sqrt{2(n+1)}\,\psi_{n+1} \end{cases}$$





0 NODES

1 NODE

2 NODES

(SIMPLE HAR OSC.)

TL

- MATRIX ELEMENT

$$\langle n|V|m\rangle = \int_{-\infty}^{\infty} \psi_n^* \, V \, \psi_m \, d\xi$$

V = PERTURBATION

- FERMI'S GOLDEN RULE

SCRÖ'S EQ'N (TIME DEPENDENT) $H\psi = \frac{i}{\hbar}\frac{\delta\psi}{\delta t}$.

PERTURB WITH A POTENTIAL V

$$\psi_i = \sum_n a_n(t)\,\phi_n(t)\, e^{-i\hbar/E_n t}$$

ψ_i = PERTURBED WAVE FUNCTION

ϕ_n = UNPERTURBED WAVE FUNCTION

GIVES: $\frac{\delta a_s}{\delta t} = \frac{-i}{\hbar}\sum_n a_n V_{sn}\, e^{i/\hbar(E_s - E_n)t}$

WHERE $V_{SN} = \langle s|V|n\rangle$

ASSUMPTIONS:

1. $\Delta a_s(t) \simeq 0 \Rightarrow a_n(0)$
2. V IS TIME INDEPENDENT
3. SYSTEM INITIALLY IS IN STATE $n \Rightarrow a_n = 1$

THEN $a_s(t) = \frac{-i}{\hbar}\int_0^t V_{SN}\, e^{i/\hbar(E_s - E_n)t}\,dt$

$= -V_{SN}\left(e^{i\hbar(E_s-E_n)t} - 1\right)/(E_s - E_n)$

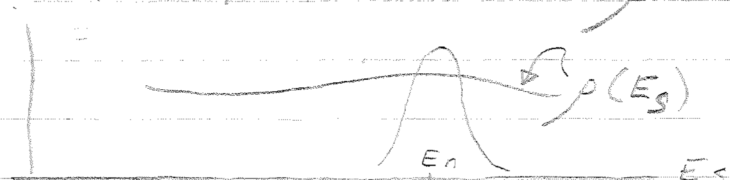
$|a_s(t)|^2 = P_s = P[\text{OF BEING IN STATE } s \text{ AT } t]$

$= 4|V_{SN}|^2 \sin^2[t/2\hbar(E_s - E_n)]/(E_s - E_n)^2$

$P(t) = \sum_s P_s(t) \hat{=} \int_s 4|V_{SN}|^2 \frac{\sin^2(\;)}{(\;)^2}\rho(E_s - E_n)\,d(E_s - E_n)$

OVER REGION OF INTEREST, $\rho(E_s - E_n)$

= DENSITY OF STATES $\simeq \rho(E_n)$

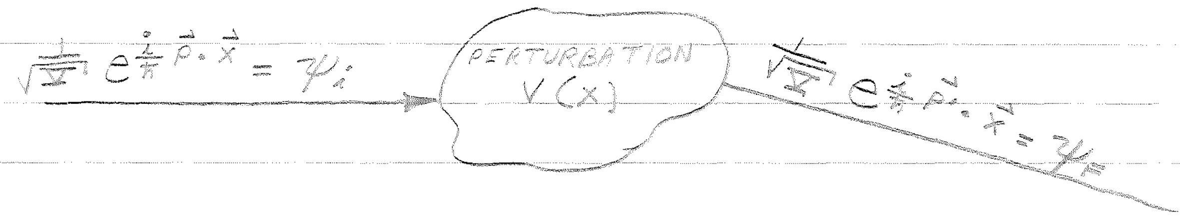


GIVES $P(t) \simeq \frac{2\pi}{\hbar}|V_{sn}|^2\rho(E_n)\,t$

$\frac{dP(t)}{dt} = \frac{2\pi}{\hbar}|V_{SN}|^2\rho(E_n)$ ← FERMI'S GOLDEN RULE #2

II FERMI'S GOLDEN RULE

● RUTHERFORD SCATTERING



DUE TO ENERGY CONSERVATION $|\vec{p}\,| = |\vec{p}\,'|$

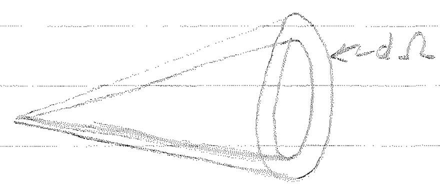
$$V_{fi} = \frac{1}{V}\int V(x)\, e^{i/\hbar(\vec{p}-\vec{p}\,')\cdot\vec{x}}\, d^3x$$

$$= \frac{1}{V}\mathcal{F}[V(x)] \Leftarrow \text{FOURIER TRANSFORM} = \frac{1}{V}\mathcal{V}(f)$$

$$\rho(E_n) = \frac{Vp^2}{(2\pi\hbar)^3}\,\frac{dP\,d\Omega}{dE} \Leftarrow \text{ASSUME}$$

$$\frac{dP(t)}{dt} = \frac{v\,d\Omega}{V}\times\frac{d\sigma}{d\Omega} \Leftarrow \text{ASSUME}$$

$d\Omega$ = SOLID ANGLE CROSS-SECTION



$d\sigma$ = FRACTION OF PARTICLES GOING INTO $d\Omega$

$$\Rightarrow \frac{dP(t)}{dt} = \frac{2\pi}{\hbar}\left|\frac{1}{V}\mathcal{V}(f)\right|^2 \frac{Vp^2\,d\Omega}{8\pi^3\hbar^3 v}$$

GIVES

$$\frac{d\sigma}{d\Omega} = \frac{1}{4\pi^2\hbar^2}\,\frac{p^2}{v^2}\left|\mathcal{V}_{pp'}(f)\right|^2$$

• FOR A COULOMB POTENTIAL

$$V(r) = zZe^2/r$$

$$\mathcal{V}_{p-p'} = zZ\int \frac{1}{r}\, e^{i/\hbar(\vec{p}-\vec{p}\,')\cdot\vec{x}}\, d^3x$$

$$= \pi\hbar^2 zZ\,\frac{e^2}{4p^2\sin^2\theta/2}$$

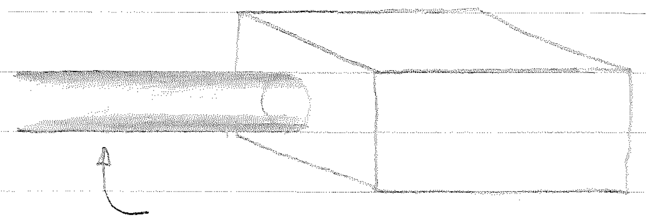
WHICH GIVES

$$\frac{d\sigma}{d\Omega} = \frac{z^2Z^2}{4}\left(\frac{me^2}{p^2}\right)^2\frac{1}{\sin^4\theta/2} \Leftarrow$$ SAME AS RUTHERFORD SCATTERING

● HEAT DIFFUSION EQN.

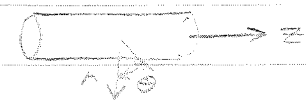
$$\nabla^2 T = \frac{\rho c}{k} \frac{\delta T}{\delta t}$$

ρ = DENSITY, C = SPECIFIC HEAT, K = THERMAL CONDUCT.



GAUSSIAN BEAM: $I = I_0 e^{-r^2/2r_0^2}$

① RADIAL DIFFUSION

USE CYLINDRICAL COOR: 

$$\Rightarrow \frac{\delta T}{\delta z} = \frac{\delta T}{\delta \theta} = 0$$

LEAVES $\frac{\rho c}{k} \frac{\delta T}{\delta t} = \frac{1}{r} \frac{\delta}{\delta r} r \frac{\delta T}{\delta r}$

USING SEPERATION OF VARIABLES: $T(r,t) = T_r T_t$

$$\Rightarrow \frac{1}{r} \frac{\delta}{\delta r} r \frac{\delta T_r}{\delta r} = -\upsilon^2 T_r \Leftarrow \text{BESSEL'S EQN.}$$

$$\frac{\rho c}{k} \, \delta T_t / \delta t = -\upsilon^2 T_t$$

GIVES $T_t = C e^{-\upsilon^2 kT/ec}$, $T_r = A_1(\upsilon) J_0(r\upsilon)$

OR $T = T_r T_t = A(\upsilon) J_0(r\upsilon) e^{-\upsilon^2 kT/ec}$

BOUNDRY CONDITIONS: $T(r,0) = T_0 e^{-r^2/2r_0^2}$

$$\Rightarrow e^{-r^2/2r_0^2} = \int_0^\infty A(\upsilon) J_0(\upsilon r) d\upsilon \Leftarrow \text{HANKLE XFORM}$$

$$\Rightarrow A(\upsilon) = \int_0^\infty r\,dr\, e^{-r^2/2r_0^2} J_0(\upsilon r)$$

$$\Rightarrow T(r,t) = \int_0^\infty \upsilon\, d\upsilon \int_0^\infty x\,dx\, J_0(\upsilon x) e^{-\frac{x^2}{2r_0^2}} dx \times e^{-\upsilon^2 kT/\rho c} J_0(\upsilon r) dr$$

$$= T_0 \alpha\, e^{-\frac{\alpha r^2}{2r_0^2}} \Rightarrow \alpha = \left(1 + \frac{2kt}{\rho c r_0^2}\right)^{-1}$$

NOTE: @ $r = 0$, $\frac{2kT}{r_0^2 \rho c} = 1 \Rightarrow 2kT = r_0^2 \rho c$

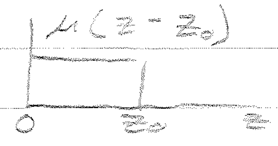
② DIFFUSION IN Z DIRECTION

$$\frac{dT}{d\theta} = 0, \quad \frac{\delta T}{\delta r} = 0$$

USING SEPERATION OF VARIABLES

$$\frac{1}{T_z}\frac{\delta^2 T_z}{\delta z^2} = -U^2 = \frac{1}{T}\frac{\delta c}{K}\frac{\delta T_t}{\delta t}$$

GIVES: $T(z) = A(U)\cos(Uz)\, e^{-U^2KT/\rho c}$



BOUNDRY CONDITION

$$T(0,t) = T_0\,\mu(z - z_0)$$

$$T(0,t) = \int_0^{\infty} A(U)\cos Uz\, dU \Leftarrow \text{FOURIER XFORM}$$

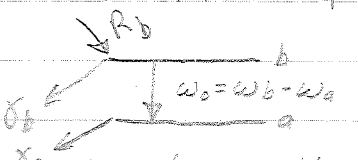
$$\Rightarrow A(U) = \frac{2}{\pi}\int_0^{\infty} T(0,z)\cos(Uz)\,dz$$

AND $T(z,t) = \int_0^{\infty} A(U)\cos(Uz)\, e^{-\frac{U^2KT}{\rho c}}\, dU$

$$= \frac{T_0}{2}\sqrt{\frac{\rho c}{\pi K T}}\int_0^{z_0} e^{-(x+z_0)\left(\frac{\rho c}{4kt}\right)} + e^{-(x-z)^2\rho c/4kT}\, dx$$

$$T(z,0) = \frac{2T_0}{\sqrt{\pi}}\int_0^{z_0\sqrt{\frac{\rho c}{4KT}}} e^{-U^2}\, dU = T_0\,\mathrm{erf}\left(z_0\sqrt{\frac{\rho c}{4kT}}\right)$$

● TWO STATE QUANTUM SYSTEM



$H = H_0 + V$ = HAMILTONIAN

H_0 = HAMILTONIAN W/ KNOWN SOLN., V = PERTURBATION

SOLN' TO H_0: $\psi = a\phi_a e^{-i\omega_a t} + b\phi_b e^{-i\omega_a t} = a|a\rangle e^{-i\omega_a t} + b|b\rangle e^{-i\omega_b t}$

ASSUMPTIONS: ① $a = a(t)$, $b = b(t)$

② $\langle a|H_0|b\rangle = \langle a|E_b|b\rangle = E_b\,\delta_{ab}$

③ $V_{aa} = V_{bb} = 0$; $V_{ab} = V_{ba}$

WE THEN HAVE:

$\langle a|H_0 + V|\psi\rangle = \langle a|H_0|a\rangle e^{-i\omega_a t} \times a + \langle a|V|b\rangle e^{-i\omega_b t} \times b$

USING $H\psi = \frac{-i}{\hbar}\frac{\delta\psi}{\delta t}$ GIVES ($\omega_0 = \omega_b - \omega_a$):

$$\begin{cases} \dot{a} = \frac{-i}{\hbar}\, b\, V_{ab}\, e^{-i\omega_0 t} \\ \dot{b} = \frac{-i}{\hbar}\, a\, V_{ab}\, e^{-i\omega_0 t} \end{cases}$$

● APPLIED $\vec{E}$ FIELD $\Rightarrow V = eE_0 X_{ab} \cos\omega t$

$\Rightarrow \langle a|V|b\rangle = V_{ab} = e\langle a|\vec{x}|b\rangle = \mu_{ab}$ ← DIPOLE

$$\text{THEN}\begin{cases} \dot{a} = \frac{-i}{\hbar}\frac{\mu_{ab}E_0}{2}\, b\left[e^{i(\omega-\omega_0)t} + \cancel{e^{-i(\omega+\omega_0)t}}^{\text{SMALL}}\right] \\ \dot{b} = \frac{-i}{\hbar}\frac{\mu_{ab}E_0}{2}\, a\left[\cancel{e^{i(\omega+\omega_0)t}}^{\text{SMALL}} + e^{-i(\omega-\omega_0)t}\right] \end{cases}$$

● DAMPING ASSUMED: $\dot{a} = -\frac{\gamma_a}{2}a$, $\dot{b} = -\frac{\gamma_b}{2}b$

$$\text{GIVES}\begin{cases} \dot{a} = \frac{-i}{\hbar}\frac{\mu_{ab}E_0 b}{2} e^{i\Omega t} - \frac{\gamma_a}{2}a \\ \dot{b} = \frac{-i}{\hbar}\frac{\mu_{ab}E_0 a}{2} e^{-i\Omega t} - \frac{\gamma_b}{2}b \end{cases} ; \Omega = \omega - \omega_0$$

SOLUTION: $a = \alpha(t)\, e^{-\frac{\gamma_a}{2}(t-t_0)}$ $\quad b = \beta(t)\, e^{-\frac{\gamma_b}{2}(t-t_0)}$

INITIAL CONDITIONS: @ $t = t_0$, $\alpha = 1$, $\beta = 0$ (above: $\beta = 1$, $\alpha = 0$)

● POLARIZATION: P_x (STEADY STATE)

$P_x = \langle\psi|\mu|\psi\rangle = \frac{\mu^2 E_0}{2\hbar}\left[\frac{R_b n_b}{\gamma_b} - \frac{R_a n_a}{\gamma_a}\right]\frac{1}{(\omega-\omega_0)^2 + \gamma_{ab}^2}\left[(\omega-\omega_0)\cos\omega t - \gamma_{ab}\sin\omega t\right]$

n_a = # ATOMS, R_a = "PUMPING" CONSTANT, γ_a = DECAY CONTS

● P_T = PROBABILITY OF TRANSITION $= \sum_i P_i = \sum_i |\langle i|V_0|b\rangle|^2$

DECAY: $\frac{dn_b}{dt} = P_T n_b$

$n_b = n_{b0}\, e^{-t\gamma_b} \Rightarrow \gamma_b = P_T$

$\Rightarrow \gamma_b = \sum_i |\langle i|V|b\rangle|^2$

II

- BOLTZMAN TRANSPORT EQUATION

SIX-DIMENSIONAL $(\vec{x}, \vec{V})$ OR $(\vec{r}, \vec{k})$ PROBABILITY DISTRIBUTION VARYING IN TIME

$$\vec{V} \cdot \vec{\nabla}_r f + \vec{a} \cdot \nabla_V f = -(f - f_0)/\tau$$

OR $$\frac{1}{\hbar}(\nabla_K \mathcal{E}) \cdot (\nabla_r f) + \frac{\vec{E}}{\hbar} \cdot \vec{\nabla} f = -(f - f_0)/\tau$$

$$\mathcal{E} = \hbar^2 k^2 / 2m^*, \quad V = \hbar k / m^*$$

[TIME DEPENDENT
$$\frac{\delta f}{\delta t} = \frac{-(f - f_0)}{\tau} - \vec{a} \cdot \nabla_K f - V \cdot \nabla_r f \Big]$$

τ = TIME CONSTANT

f_0 = KNOWN DISTRIBUTION

1-D D.C. DISTURBANCE

$$f = f_0 - \tau\left[V_x \frac{\delta f}{\delta x} + a_x \frac{\delta f}{\delta V_x}\right]$$

- CURRENT DENSITY: J_x

$$J_x = -e \Sigma V_x = -e \int f V_x d\vec{V} \quad \left(\frac{AMP}{m^2}\right)$$

ALL KNOWN f_0 ARE EVEN WRT $V \Rightarrow \int f_0 d\vec{V} = 0$

$$\Rightarrow J_x = e \iiint_{-\infty}^{\infty} \tau \left(V_x \frac{\delta f_0}{\delta x} + a_x \frac{\delta f_0}{\delta V_x}\right) V_x \, dV_x dV_y dV_z$$

- THERMAL CURRENT DENSITY: C_x $\left(\frac{WATTS}{m^2}\right)$

$$C_x = \iiint f V_x \mathcal{E} \, dV_x dV_y dV_z$$

$$= -\iiint \tau \left(V_x \frac{\delta f_0}{\delta x} + a_x \frac{\delta f_0}{\delta V_x}\right) V_x \mathcal{E} \, dV_x dV_y dV_z$$

FOR FREE e's

- FOR MAXWELL-BOLTZMAN DISTRIBUTION (ION GAS ~~METAL~~ METAL)

$$f_0 = n\left(\frac{m}{2\pi kT}\right)^{3/2} e^{-mV^2/2kT}$$

ASSUME $$\frac{\delta f_0}{\delta x} = \left(\frac{mV^2}{2kT} - \frac{3}{2}\right) \frac{f_0}{T} \frac{\delta T}{\delta x}$$ CONST. E_x FLD

$$a_x \frac{\delta f_0}{\delta V_x} = \frac{eE_x}{kT} V_x f_0$$ UNIFORM $\frac{\delta T}{\delta x}$

$$I_0 = \int_{-\infty}^{\infty} e^{-mV_x^2 \beta/2} dV_x = \sqrt{\frac{2\pi}{m\beta}}\ ; \quad I_j = (-1)^j \frac{d^j I_0}{d\beta^j}$$

GIVES $$J_x = \frac{ne\tau}{m} \frac{\delta(kT)}{\delta x} + \frac{ne^2\tau}{m} E_x$$

$$C_x = \frac{-5n(kT)\tau}{m} \frac{\delta(kT)}{\delta x} - \frac{5ne(kT)\tau}{2m} E_x$$

τ ASSUMED CONST

II BOLTZMAN XPORT EQN

• CONDUCTIVITY

• $J_x / E_x = \sigma$ = CONDUCTIVITY = $\frac{n e^2 \tau}{m} = e \mu n$

FROM $\frac{\delta T}{\delta x} = 0$

• $K = C_x \Big/ \delta T / \delta x \Big|_{J_x = 0} = \frac{5 n^2 k^2 T \tau}{2m}$

= THERMAL CONDUCTIVITY

• $\frac{K}{\sigma T} = 5k^2 / 2e^2$

• THERMAL ELECTRIC → J_x FLOWS, (NO E) DUE TO T DIFFERENCE

• FERMI (DEGENERATE GASSES) (METAL

$f(\varepsilon) = \left[1 + e^{(\varepsilon - \varepsilon_F)/kT} \right]$ $\quad \varepsilon = \frac{\hbar^2 k^2}{2m^*}$

GIVES $\sigma = \frac{e^2 n}{m^*} \tau(\varepsilon_F)$

$K = \frac{\pi^2}{3} \frac{k^2}{m^*} n \tau(\varepsilon_F)$

$\frac{K}{\sigma T} = \frac{\pi^2}{3} \left(\frac{k^2}{e} \right)^2$ ⇐ WIEDEMANN-FRANZ RATIO

II BOLTZMANN VPORT EQN.

TEST # 3 (FINAL) STUDY SHEET

1. BAND STRUCTURE CALCULATION
   BORN-OPPENHEIMER | HARTRE-FOCK | LCOA
2. BLOCH FUNCTIONS
2. K·P APPROXIMATION
3. BAND TO BAND TRANSITION
4. LIGHT ABSORBTION (REFR. INDEX
5. ABSORBTION COEFFICIENTS
5. P-N JUNCTION
6. NPN BJT
7. NPN BJT (CONT)
7. JFET
8. IMPURITY SCATTERING

III

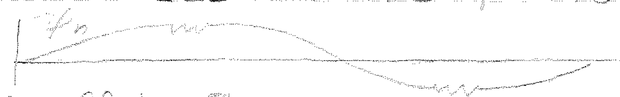
BAND-STRUCTURE CALCULATION

ACTUAL HAMILTONIAN:

$$H = -\underbrace{\sum_i \frac{\hbar^2}{2M}\nabla_i^2}_{\text{NUCLEUS}} - \underbrace{\sum_j \frac{\hbar^2}{2m}\nabla_j^2}_{\text{ELEC}} + \underbrace{\frac{1}{2}\sum_{ij}^{i\neq j}\frac{e^2}{|\vec{r}_i-\vec{r}_j|}}_{\text{ELEC/ELEC}} + \underbrace{\frac{1}{2}\sum_{K,l}^{K\neq l}\frac{Z^2e^2}{|R_K-R_l|}}_{\text{NUC/NUC}} - \underbrace{\frac{1}{2}\sum_{K,j}\frac{Ze^2}{|R_K-r_j|}}_{\text{NUC/ELEC}}$$

BORN-OPPENHEIMER APPROXIMATION

SEPARATE ELECTRONIC & VIBRATIONAL MOTION



$$\psi = \psi_e \psi_n$$

2^{ND}, 3^{RD} & 5^{TH} TERM ← FROM NUCLEUS

ASSUME $E_e = \int \psi_e^* H \psi_e = -\sum_j \int \phi_{e_j}^* \nabla_j^2 \phi_{e_j} + \frac{1}{2}\sum_{ij}\int \psi_e^* V_{ee} \psi_e$

$$V_{ee} = \frac{1}{2}\sum_{ij}^{i\neq j}\frac{e^2}{|r_i-r_j|} - \frac{1}{2}\sum_{jK}\frac{Ze^2}{|R_K-r_j|}$$

$$\Rightarrow E_e = \sum_j E_j + \frac{1}{2}\sum_{ij}\phi_j^*\phi_i^* V_{ij}\phi_j\phi_i \; : \; V_i = \frac{e^2}{|r_i-r_j|}$$

GOOD FOR ONLY ONE ELECTRON:

$$\left[H_j + \frac{1}{2}\sum_{i\neq j}\int\frac{e^2}{|r_i-r_j|}\phi_i^*\phi_i\right]\phi_j = E_j\phi_j \Leftarrow \text{HARTREE EQN.}$$

HARTREE-FOCH APPROX. (SLATER DETERMINENT)

ASSUME: (1) N ELEC, 1 IN OUTER SHELL (2) SPHER. SYM. (3) SELF CONSISTANCY

HARTREE ASSUMPTION: $\psi = \phi_1\phi_2\ldots\phi_N$; $\phi_n = n^{TH}$ e^- WAVE FUNCT.

HARTREE FOCH INCLUDED EXCHANGE TERMS:

$$\psi(x) = \frac{1}{N!}\begin{vmatrix}\phi_1(x_1) & \phi_1(x_2) & \cdots \\ \phi_2(x_1) & & \\ \vdots & & \phi_n(x_n)\end{vmatrix} \Leftarrow \text{SLATER DETERMIN.}$$

$$= \frac{1}{\sqrt{2}}\left(\phi_1(x_1)\phi_2(x_2) - \phi_1(x_2)\phi_2(x_1)\right) \Leftarrow N = 2$$

$$\phi_1(x_1) = \phi_{1(SPACE)}(x_1)\,\phi_{1(SPIN)}\,(m = \pm\tfrac{1}{2})$$

WISH TO DESYMMETERIZE WAVE FUNCTION

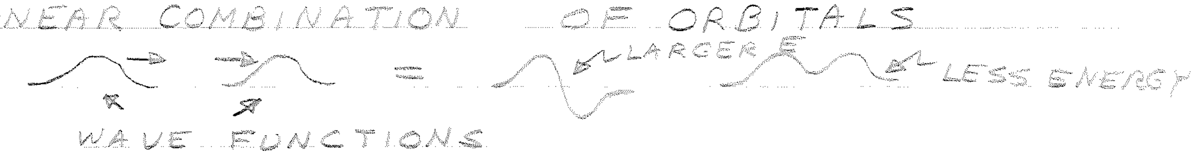
$$\psi = \frac{1}{\sqrt{2}}\left[\phi_{1SPA}^{(x_2)}\phi_{2SPA}^{(x_1)} - \phi_{1SPA}^{(x_1)}\phi_{2SPA}^{(x_2)}\right]\left[\phi_{1SPIN}^{(1)}\phi_{2SPIN}^{(2)} - \phi_{1SPI}^{(2)}\phi_{2SPI}^{(1)}\right]$$

RESULTING ENERGY IS

$$E = \sum_i \int \phi_i^*\left(-\frac{\hbar}{2m}\nabla_i^2\right)\phi_i + \sum_{ij}\left[\phi_i^*(x_1)\phi_j^*(x_2)\left[\frac{e^2}{4\pi\epsilon|x_i-x_j|}\right]\right. \leftarrow \text{POT ENER}$$

$$\times\left[\phi_i(x_1)\phi_j(x_2) - \delta_{m_{SPIN\,i},\,m_{SPIN\,j}}\,\phi_i(2)\phi_j(1)\right]dx_2\,dx_1$$

LINEAR COMBINATION OF ORBITALS



III

BAND STRUCTURE: BORN-OPPEN / HARTREE-FOCH / LCOA/SLATER

- BLOCK FUNCTIONS (ELECTRON IN A CRYSTAL)

$v(\vec{r})$ 

PERIODIC PROPERTY: $|\psi_{\vec{k}}(x)|^2 = |\psi_{\vec{k}}(x+a)|^2$

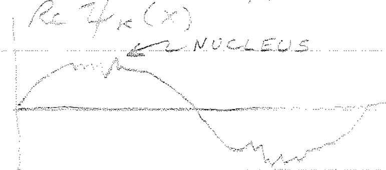
TAYLOR SERIES: $\psi(x+x_0) = \psi|_{x_0} + \frac{\delta \psi}{\delta x}\Big|_{x_0} x + \frac{1}{2!}\frac{\delta^2 \psi}{\delta x^2}\Big|_{x_0} x^2 + \ldots$

$$= e^{x \frac{\delta}{\delta x}}\, \psi(x_0)$$

RECALL $\frac{\hbar}{i}\frac{\delta}{\delta x} \Leftrightarrow \vec{p} \Leftrightarrow \hbar \vec{k}$

$$\Rightarrow \psi(x+x_0) = \psi(x_0)\, e^{i x \cdot k_x}$$

$\psi_{\vec{k}}(\vec{x}+\vec{x}_0) = U_{\vec{k}}(\vec{x})\, e^{i \vec{k}\cdot\vec{x}}$ ⇐ IN 3-D

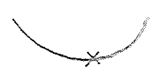


- k·p APPROXIMATION (USING BLOCK FUNCTIONS)

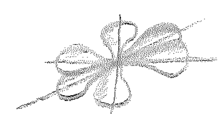
$\left[\frac{-\hbar^2}{2m}\nabla^2 + V\right] U_{\vec{k}}(\vec{r})\, e^{i\vec{k}\cdot\vec{r}} = E(\vec{k})\, U_{\vec{k}}(\vec{r})\, e^{i\vec{k}\cdot\vec{r}}$ ⇐ SCHÖ'S EQ FOR ELEC. IN A CRYSTAL

GIVES $\left[\frac{\vec{p}^{\,2}}{2m} + \frac{\hbar}{m}\vec{k}\cdot\vec{p} + \frac{\hbar^2 k^2}{2m}\, V\right] U_{\vec{k}}(\vec{r}) = E(\vec{k})\, U_{\vec{k}}(\vec{r})$

APPLICATION TO GERMANIUM (DIRECT GAP, SMALL $\vec{k}$)

 ← CONDUCTION BAND (SPREAD S STATE)

 ← VALENCE BAND (P STATE: 3 STATES:) (6 STATES W/ SPIN)



$U_k = a_c U_c + a_v U_v = \sum_{i=1}^{4} a_{ki} U_i$

ONE FUNCTION ($a_c U_c$) TWO FUNCTIONS ($a_v U_v$)

GIVES $0 = \sum_{i=1}^{4} \left\{ E_i + \frac{\hbar}{m} k\cdot p - E(k) \right\} a_{ki} U_i(\vec{r})$

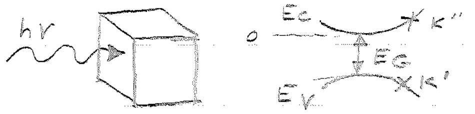
FOR SMALL K, $U_i \perp U_j$. $P = \langle U_i | P_x | U_j \rangle$ = MATRIX ELEMENT DIPOLE MOMENT

GIVES $\begin{vmatrix} E_c - E(\vec{k}) & k_x P & k_y P & k_z P \\ k_x P & E_v - E(\vec{k}) & 0 & 0 \\ k_y P & 0 & E_v - E(k) & 0 \\ k_z P & 0 & 0 & E_v - E(\vec{k}) \end{vmatrix} = 0 \Rightarrow E(\vec{k}) = \begin{cases} E_v \\ E_v \\ \frac{E_c + E_v}{2} + \sqrt{\left(\frac{E_c - E_v}{2}\right)^2 + k^2 P^2} \\ \frac{E_c + E_v}{2} - \sqrt{\left(\frac{E_c - E_v}{2}\right)^2 + k^2 P^2} \end{cases}$

FOR SMALL $\vec{k}$: $E(\vec{k}) \simeq E_c \pm \frac{2 k^2 P^2}{E_c - E_v}$ ← PARABOLIC (FREE LIKE e^-)

III

- BAND TO BAND TRANSITION (NON-DEGENERATE)



$$E_V(\vec{k}') = -E_G - \frac{\hbar^2}{2m_h^*} k'^2$$
$$E_C(k'') = \frac{\hbar^2 k''^2}{(2m_e^*)}$$

$$\hbar\omega = E_C(k'') - E_V(k')$$

ψ_0 = VAL. BAND = $\frac{1}{\sqrt{N}} U_V(\vec{r}, \vec{k}') e^{i\vec{k}'\cdot\vec{r}}$; ψ_m = COND BAND = $\frac{1}{\sqrt{N}} U_C(\vec{r}, \vec{k}'') e^{i\vec{k}''\cdot\vec{r}}$

APPLIED $\vec{H}$ FIELD: $\vec{\nabla}\times\vec{A} = \vec{H}$; $\nabla\cdot A = 0$ A = MAGNETIC POTENTIAL

$$\vec{p} = i\hbar\nabla + \frac{eA}{c} \Rightarrow \frac{p^2}{2m} = \frac{-\hbar^2}{2m}\nabla^2 + \frac{i\hbar e}{mc}\vec{A}\cdot\vec{\nabla} + \frac{e^2|A|^2}{2mc^2} \to \text{SMALL}$$

FOR $A\cdot\nabla >> |A|^2$, PERTURBATION = $H'(\vec{r}) = \frac{i\hbar e}{mc}\vec{A}\cdot\vec{\nabla}$

$$\vec{A} = a_0 A\cos(\vec{K}\cdot\vec{r} - \omega t) ; |\vec{K}| = \frac{\omega r}{c} \Rightarrow r = Re(r^*)$$

FERMI POTENTIAL: $H'(\vec{r}) = \frac{ie\hbar}{2mc} A e^{i(\vec{K}\cdot\vec{r}-\omega t)} \hat{a}_0\cdot\vec{\nabla} + \text{c.c.}$

RATE OF TRANSITION: $P \cong \frac{4|H_{k'k''}|^2 \sin^2[(E_{k''} - E_{k'} - \hbar\omega)\frac{t}{2\hbar}]}{(E_{k''} - E_{k'} - \hbar\omega)^2}$

- MATRIX ELEMENT:

$$H_{k'k''} = \frac{ie\hbar A}{2Nmc}\int_{\substack{ALL\\STATES}} U_C^*(\vec{r},\vec{k})\Big[\underbrace{\vec{a}_0\cdot\vec{\nabla}U_V(\vec{r},\vec{k})}_{\substack{\text{ALLOWED}\\\text{DIRECT XSITION}}} + \underbrace{i(\vec{a}_0\cdot\vec{k})U_V(r,k)}_{\substack{\text{FORBIDDEN}\\\text{DIRECT XSITION}}}\Big] e^{i(k'+\vec{K}-k'')\cdot\vec{r}} d^3r$$

FOR $\vec{k}''-\vec{k} = \epsilon$ SMALL $\underbrace{\int U_V U_C^* e^{i\epsilon r} \cong 0}_{\text{ALLOWED}}$ SINCE $\underbrace{\int U_V U_C^* = 0}_{\text{FORBIDDEN}}$

$$H_{k'k''} = \frac{ie\hbar A}{2mc}\int_{\substack{UNIT\\CELL}} U_C^*(\vec{r},k'')\left[\hat{a}_0\cdot\nabla U_V(r,k') + i(\hat{a}_0\cdot k')U_V(r,k')\right]d^3r$$

- (ALLOWED) TRANSITION $P_r = \underbrace{P(E)}_{\text{DENS. STATE}} t = \frac{e^2A^2}{4\pi^3 m^2c^2}\int|\hat{a}_0\cdot P_{k''k'}|^2 \frac{\sin^2[(E_{k''}-E_{k'}-\hbar\omega)\frac{t}{2\hbar}]}{(E_{k''}-E_{k'}-\hbar\omega)^2} d^3k'$

WHERE: $H_{k''k'}^{\text{ALLWED}} = \frac{-eA}{2mc}(\hat{a}_0\cdot\vec{P}_{k'',k})$; $P_{k''k'} = i\hbar\int_{CELL} U_C(\vec{r},k'')\nabla U_V(r,k')d^3r$

$$d^3k' = k'^2 dk' d\Omega \Rightarrow \int|\hat{a}_0\cdot P_{k''k}|^2 d\Omega = 4P\,\overline{P_{k'k''}}$$

$$\Rightarrow P(E)t = \frac{e^2A^2}{(\pi mc)^2}\int \overline{P_{k''k}}^2 \frac{\sin^2[(E_{k''}-E_{k}-\hbar\omega)\frac{t}{\hbar\omega}]}{[E_{k''}-E_{k'}-\hbar\omega]^2} k'^2 dk'$$

$$= \frac{e^2A^2\sqrt{2m_r}}{4\pi m^2c^2\hbar^4}\overline{P_{k''k}}^2\sqrt{\hbar\omega - E_G} ; m_r = \frac{m_e m_h}{m_e + m_h}$$

- ABSORBED PHOTONS = INCIDENT PHOTONS $\times e^{-\alpha d}$

$\alpha = \frac{P(E)\hbar\omega}{|\vec{S}|}$ FOR $\alpha d << 1$; $S = \frac{c}{4\pi}\vec{E}\times\vec{H} = \frac{A^2 k\omega}{8\pi}$

- OSCILLATOR STRENGTH: $f_{k''k'} = \frac{2|\overline{P_{k''k'}}|^2}{m\hbar\omega} \cong 1 + \frac{m_e}{m_h^*}$ FOR $V \to C$ IN SEMI

ALLOWED: $\alpha = \frac{2\times10^5}{r}\left(\frac{2m_r^*}{m}\right)^{3/2} f(\hbar\omega - E_G)^{\frac{1}{2}}$

FORBIDDEN: $f' = \left|\int_{\substack{CELL\\UNIT}} U_C^*(r,k'')U_V(r,k')d^3r\right|^2$

$P(E) = \frac{e^2A^2(2m_r^*)}{12\pi m^2\hbar^4} f'(\hbar\omega - E_G)^{3/2}$, $\alpha = \frac{1.8\times10^5 f'}{r\hbar\omega}\left(\frac{2m_r^*}{m}\right)^{5/2}(\hbar\omega - E_G)^{3/2}$

3 ORDERS OF MAG DIFFERENCE IN α'S

- LIGHT ABSORBTION IN A SOLID (REFR. INDEX)

$$\frac{\delta^2 \mathcal{E}}{\delta x^2} - \frac{\epsilon}{c^2}\frac{\delta^2 \mathcal{E}}{\delta t^2} = \frac{4\pi\sigma}{c^2}\frac{\delta \mathcal{E}}{\delta t} \Leftarrow \text{FROM MAXWELL}$$

μ = PERMITTIVITY ; ϵ = DIELECTRIC CONSTANT ; $c = \frac{1}{\sqrt{\mu\epsilon}}$

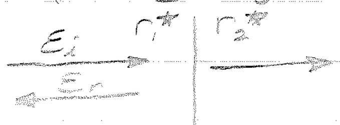
$$\mathcal{E} = A e^{i(kx-\omega t)} \Rightarrow \frac{k^2}{\omega^2} = \frac{\epsilon}{c^2} + \frac{i4\pi\sigma}{\omega c^2} = \frac{1}{(V^*)^2}$$

REFRACTIVE INDEX: $r^* = \frac{c}{V^*} = \sqrt{\epsilon + \frac{i4\pi\sigma}{\omega}} = r(1+i\gamma)$

$$r = \frac{1}{\sqrt{2}}\left[\epsilon + \sqrt{\epsilon^2 + \frac{16\pi^2\sigma^2}{\omega^2}}\right]^{1/2} ; \quad \gamma = \sqrt{1 - \epsilon/r^2}$$

BEER ABSORBTION: $dI = -\alpha(1-r)I\,dx$

$$\alpha = \frac{2\omega}{c} r\gamma = \frac{4\pi}{cr}\sigma$$; α = ABSORBTION COEFF



$\mathcal{E} \sim Y$ POLARIZED

$H \sim Z$ POLARIZED

$$\begin{Bmatrix} \mathcal{E}_i = \mathcal{E}_{i0} e^{ikr_1^*} \\ H_i = r_1^* \mathcal{E}_i \end{Bmatrix} \begin{Bmatrix} \mathcal{E}_T = \mathcal{E}_{T0} e^{ikr_2^*} \\ H_T = r_2^* \mathcal{E}_T \end{Bmatrix} \begin{Bmatrix} \mathcal{E}_r = \mathcal{E}_{r0} e^{ikr_1^*} \\ H_r = -r_1^* \mathcal{E}_r \end{Bmatrix}$$

BOUNDRY CONDITIONS: $\mathcal{E}_{i0} = \mathcal{E}_{t0} + \mathcal{E}_{r0}$; $r_1^* \mathcal{E}_{i0} = r_2^* \mathcal{E}_{t0} - r_1^* \mathcal{E}_r$

GIVES $\frac{\mathcal{E}_{r0}}{\mathcal{E}_{t0}} = \frac{r_2^* - r_1^*}{r_2^* + r_1^*}$

R = REFLECTION COEFFICIENT $= \left|\frac{\mathcal{E}_{r0}}{\mathcal{E}_{t0}}\right|^2 = \frac{(r_2-r_1)^2 + (r_2\gamma_2 - r_1\gamma_1)^2}{(r_2+r_1)^2 + (r_2\gamma_2 + r_1\gamma_1)^2}$

FOR A METAL (HI σ): $R \simeq 1 - \frac{2}{\sqrt{2\pi\sigma/\omega}}$

$$\sigma = \frac{ne^2}{m_e^*}\left\langle \frac{\tau}{1+\omega^2\tau^2} \right\rangle_E ; \quad \sigma_{\omega\to 0} = \frac{ne^2\langle\tau\rangle}{m_e^*}$$

$$\alpha = \sqrt{\frac{8\pi}{c^2}}\,(\sigma_0\omega)^{\frac{1}{2}} \Leftarrow \text{ABSORBTION COEFF}$$

FOR A METAL: $\omega\tau \ll 1$ (LOTSA FREE e^-)

FOR AN INS (SEMICOND): $\omega\tau \gg 1$

$$\sigma = \frac{ne^2}{m_e^*\omega}\left\langle \frac{1}{\tau} \right\rangle , \quad \alpha = \frac{ne^2\lambda^2}{\pi m_e^* r c^3}\langle\tau\rangle$$

- ABSORBTION COEFFICIENTS

DIRECT ALLOWED XSITION: $\alpha \propto \sqrt{\hbar\omega - E_g}$

DIRECT FORBIDDEN XSITION: $\alpha \propto \frac{1}{\hbar\omega}(\hbar\omega - E_g)^{3/2}$

INDIRECT TRANSITIONS:

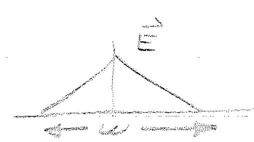
ALLOWED: $\alpha \propto \frac{(\hbar\omega \pm \hbar\omega_{PHONON} - E_g)^2}{e^{\hbar\omega_{PHO}/KT} - 1}\left[e^{-\hbar\omega_{PHO}/KT}\right]$ ← ONLY FOR "−" SIGN

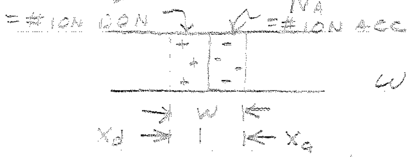
FORBIDDEN: $\alpha \propto \frac{(\hbar\omega \pm \hbar\omega_{PHO} - E_G)^3 \, e^{\hbar\omega_{PH}/KT}}{e^{\hbar\omega_{PH}/KT}}$

$\vec{K}_{VAL} = \vec{K}_{PHO} + \vec{K}_{COND}$

INDIRECT TRANSITION

- P-N JUNCTION





W = DIFFUSION LENGTH

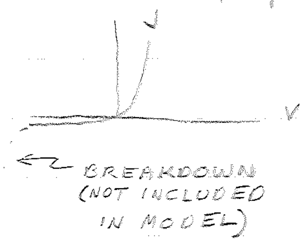
$$w = x_d + x_a = \sqrt{\frac{2\epsilon KT}{e^2}\ln\frac{N_a N_d}{n_i^2}\left(\frac{1}{N_A}+\frac{1}{N_D}\right)}$$

$V_d = \frac{KT}{e}\ln\frac{N_a N_D}{n_i^2}$; $w(V) = \text{CONS} \times \sqrt{V}$

$n_p = n_n e^{-eV_d/KT} \xrightarrow{BIAS} n_p = n_n e^{-[e(V_d+V)]/KT}$

$p_n = p_p e^{-e(V_d+V)/KT}$ W/BIAS

$J = \text{CONST}\,[(n_p+p_n)] + (n_n+p_p) = J_{SO}\left[e^{qV/KT} - 1\right]$

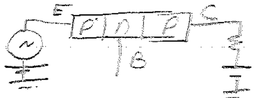


LINEARIZING:

$J = J_{SO}\left[1 + \frac{qV}{KT} + \dots\right]$

$\approx \frac{qVJ_{SO}}{KT}$ FOR $\frac{qV}{KT} \ll 1$

- PNP BJT TRANSISTOR



$I_E \sim I_C$ $P_{GAIN} \sim \frac{R_L}{R_{IN}}$

$I_{nc} << I_{PE}$, $I_{nc} << I_{PE}$

$$J = q\left[\frac{D_p P_{no}}{L_p} + \frac{D_n}{L_n n_{po}}\right]\left[e^{qV/KT} - 1\right]$$

D_n = DIFF CONST FOR e — L_p = MEAN FREE h PATH

D_p = " " " HOLES — P_{no} = EQUALIBRIUM h CONC. ON n

L_n = MEAN FREE e^- PATH — n_{po} = " e " " p

n_p = # e^- ON p WHEN V_a IS ON — n_n = CONC. OF e^- ON n SIDE

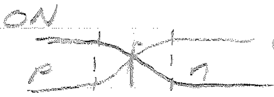
BOLTZMAN APPROX: $P_n = P_{no} e^{qV_a/KT}$; $n_p = n_{no} e^{qV_a/KT}$

ASSUMPTIONS: ① ABRUPT DEPLETION LAYER

② BOLTZMAN APPROX ③ CONST. e & h CURRENT

④ LOW LEVEL INJECTION

e/h DENSITY



Ⓘ CONTINUITY: $\frac{dn}{dt} = G - \frac{n - n_o}{\tau_n} + \frac{1}{q}\vec{\nabla}\cdot\vec{J}$ ⇐ e CURRENT

$\frac{dP}{dt} = G - \frac{P - P_o}{\tau_P} - \frac{1}{q}\vec{\nabla}\cdot J$ ⇐ h CURRENT

G = RATE OF GENERATION OF EXESS e-h PAIRS, $n - n_o$ = EXCESS CARRIER DENSITY

Ⓘⓘ CURRENT EQ: FROM BOLTZMAN XPORT EQ.

$J_n = q\mu_n n\vec{E} + qD_n\vec{\nabla}n$; $J_p = q\mu_p n\vec{E} - qD_n\vec{\nabla}p$

$\mu = \frac{q}{m^*}\frac{\langle v^2\tau\rangle}{\langle v^2\rangle}$, $D = \frac{\langle v^2\tau\rangle}{3}$ $D_n = \frac{KT}{q}\mu_n$

Ⓘⓘⓘ COMBINING: $D_n\frac{\delta^2 n}{\delta x^2} + \mu_n\left[E\frac{dn}{dx} + \cancel{\frac{n\,dE}{dx}}\right] - \frac{n - n_o}{\tau_n} = 0$ | $D_p\frac{d^2p}{dx^2} - \mu_p\left[E\frac{dp}{dx} + \cancel{\frac{p\,dE}{dx}}\right] - \frac{P}{\tau}$ NEGLECT NEGLECT

CHARGE NEUTRALITY: $\frac{n - n_o}{\tau_n} = \frac{P - P_o}{\tau_P}$

Ⓘⓥ ASSUME LL INJECTION ⇒ $\frac{\delta^2 P}{\delta x^2} - \frac{P - P_{no}}{D_p\tau_p} = 0$

$L_p = \sqrt{D_p\tau_p}$ ⇒ $P - P_{no} = P_{no}e^{-x/L_p}\left[e^{\frac{qV_a}{KT}} - 1\right]$

$J_p = q\frac{D_p P_{no}}{L_p}\left(e^{qV_a/KT} - 1\right)$ ← HOLE CURR. DENS. FOR AN JUNC.

$J_n = q\frac{n_{po}D_n}{L_n}\left[e^{qV_a/KT} - 1\right]$

ⓥ $J = J_{so}\left[e^{qV_a/KT} - 1\right] \ni J_{so} = \frac{q n_{po} D_n}{L_n} + \frac{q P_{no} D_p}{L_p}$

III

B.C.: $P(x=0) = P_{no}\, e^{qV_E/kT}$, V_E = EMIT/BASE

INTO IV ⟹ $P(x) = p(x=0)\sinh\left(\frac{W_B - x}{L_p}\right)/\sinh(W_B/L_p)$

$J_p = -qD_p \frac{\delta P}{\delta x}$, $J_p|_{EM}(x=0) = qP(x=0)\frac{D_p}{L_p}\frac{\cosh(W_B/L_p)}{\sinh(W_B/L_p)}$

$J_p|_{COLL} = qp(x=0)\frac{D_p}{L_p}/\sinh(W_B/L_p)$

CRITICAL ⟹ $\frac{W_B}{L_p}$ MUST BE SMALL

- I IN E: $\frac{I_E}{a} = \frac{qD_n n_n}{L_n}(e^{qV_E/kT}-1)$ ← e^- CUR ← E HOLE CURRENT

  $+\ qP_n(x=0)\frac{D_p}{L_p}\frac{qV_E}{kT}\frac{\cosh W_B/L_p}{\sinh W_B/L_p}$

- I IN C: $\frac{I_C}{a} = \underbrace{\frac{qD_n n_{pc}}{L_n}}_{C\ e\ cur} + \underbrace{qP_n(x=0)e^{qV_E/kT}}_{C\ h\ cur}\frac{D_p}{L_p}/\sinh\left(\frac{W_B}{L_p}\right)$

n_{pc} = EQUALIBRIUM VALUE OF IN ~~P~~ COLL.

- $\alpha = \gamma B \alpha^* = \frac{dI_C}{dI_E}$

  $\gamma = dI_E(HOLE)/\delta I_E(TOTAL) = \left[1+\frac{D_n L_p n_{p1}}{D_p L_n p_{n2}}\frac{\cosh(W_B/L_p)}{\sinh(W_B/L_p)}\right]^{-1}$

  = EMISSION EFF. OF FRAC OF EMITTED HOLE CURR

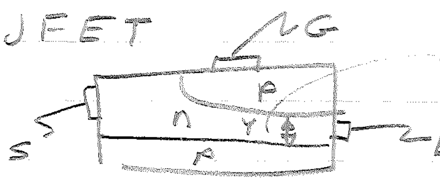
  $B = dI_C(HOLES)/dI_E(HOLES) = 1/\cosh W_B/L_p$

  = BASE XPORT FACTOR = FRAC EMITTED HOLES THAT MAKE IT TO COLLECTOR

  α^* = RATIO OF COLL. CURR TO INC. HOLE CURR.

  $\approx \frac{\sigma(MAJ)}{\sigma(MIN)} + 1 \approx 1$

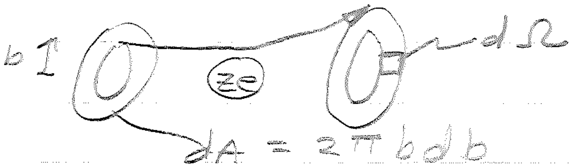
- JFET



σ IS FUNCTION OF WIDTH Y

$Y = \sqrt{\frac{2\epsilon}{qN_D}[V(x)+V_0-V_{GS}]}$

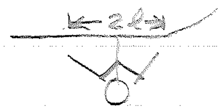
- IMPURITY SCATTERING IN SEMICONDUCTOR



b = IMPACT PARAMETER

S = SCATTERING CROSS SECTION = $\frac{2b\pi\,db}{2\pi \sin\theta\, d\theta}$

ASSUME: ①

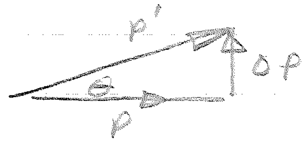


$F = Ze^2/\epsilon l^2$

② SMALL SCATTER ANGLE

③ INITIAL VELOCITY = V

$\Rightarrow \Delta p = Ze^2/bV$



SMALL ANGE: $\frac{\Delta p}{p} = \theta = \frac{Ze^2\,2}{bmV^2}$

GIVES ΔE = LOSS IN ENERGY = $\frac{(\Delta p)^2}{2m} = 2Z^2e^4/mb^2V^2$

REAL ANSWER IS

$\tan\frac{\theta}{2} = \frac{Ze^2}{bmV^2}$; $S = \left(\frac{Ze^2}{2\epsilon mV^2}\right)\frac{1}{\sin^4(\theta/2)}$