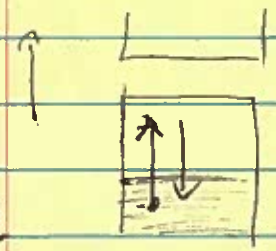
PHYS 460 - LECTURE 13

OPTICAL PROPERTIES OF SOLIDS

AS WITH ELECTRICAL PROPERTIES, MUCH OF THE PHENOMENOLOGY SURROUNDING OPTICAL PROPERTIES CAN BE UNDERSTOOD FROM THE PERSPECTIVE OF BAND THEORY. THIS IS BECAUSE OPTICAL LIGHT PRIMARILY INTERACTS WITH SOLIDS BY EXCITING ELECTRON MODES, AND WHICH ~~k~~ WAVELENGTHS (i.e ENERGIES) OF LIGHT A MATERIAL CAN ABSORB DEPENDS ON THE AVAILABILITY OF OPEN STATES.

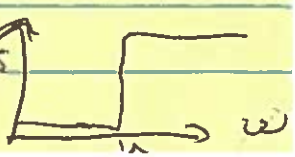
CASES: (1) METALS: ELECTRONS IN A HALF FILLED BAND ARE PROMOTED TO HIGHER ENERGIES AND THEN FALL AND REEMIT LIGHT AT (NEAR) THE SAME FREQ. (REFLECTION)



NOTE THIS IS WHY METALS ARE SHINY!

THE RANGE OF λ THAT CAN PARTICIPATE IN THIS PROCESS DEPENDS ON THE BANDWIDTH. THIS IS WHY MATERIALS WITH LARGE t (e.g SILVER) LOOK BLUER THAN MATERIALS WITH SMALLER t (e.g COPPER)

(2) INSULATORS: IDEALLY INSULATORS DON'T INTERACT WITH ANY LIGHT AT ALL UNTIL $\omega > \Delta$ AND ELECTRONS CAN BE EXCITED ACROSS THE GAP. THUS ONE USEFUL WAY OF MEASURING Δ IS THROUGH OPTICAL ABSORPTION MEASUREMENTS



(3) INSULATORS WITH IMPURITIES:

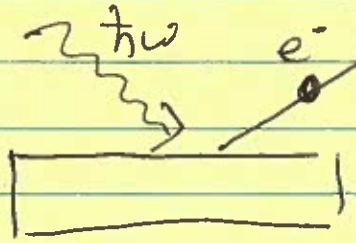
SINCE NOT MUCH ELSE IS GOING ON, THE LOOK OF INSULATORS IS STRONGLY AFFECT BY SMALL DENSITIES OF IMPURITY ATOMS (AND THEIR OWN ATOMIC TRANSITIONS)

e.g.
- 1 ppm N^{2+} TURNS DIAMOND YELLOW
- 1 ppm B^{2+} GIVES DIAMOND A BLUISH TINGE
- ALL SAPPHIRES AND RUBIES ARE FUNDAMENTALLY CRYSTALS OF Al_2O_3, ~0.1% IMPURTY ATOMS IN PLACE OF Al^{3+}

PHOTOELECTRIC EFFECT

AT HIGH ENOUGH FREQUENCIES, OF COURSE, ELECTRONS CAN BE KICKED RIGHT OUT OF THE MATERIAL, AN OBSERVATION COINED THE "PHOTOELECTRIC EFFECT", ORIGINALLY DISCOVERED BY ALEXANDRE BECQUEREL IN 1839, IT WAS NOT EXPLAINED UNTIL 1905 BY ALBERT EINSTEIN, WHO WON THE NOBEL PRIZE FOR THIS WORK (1921)

BASIC PICTURE



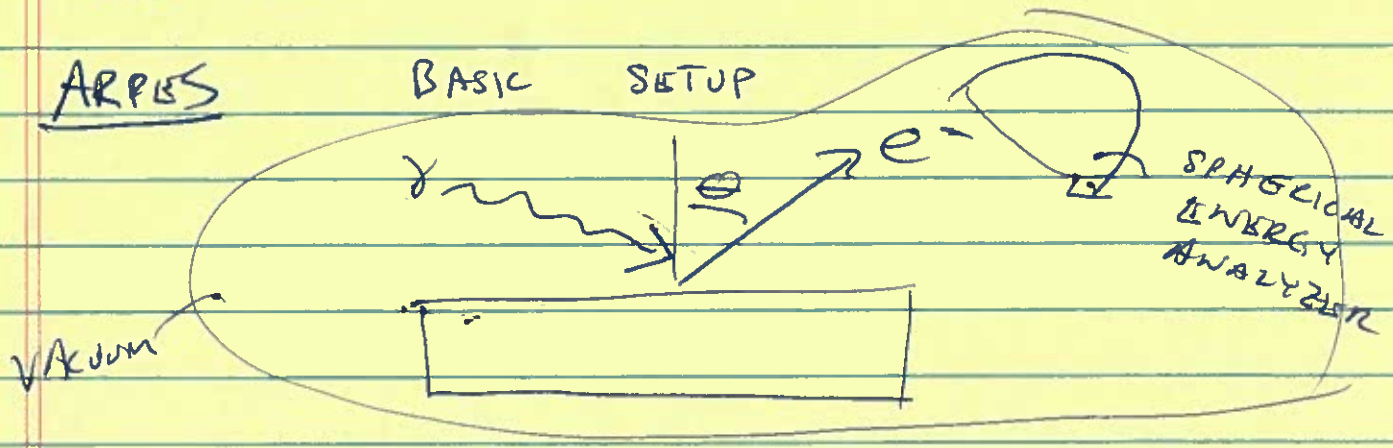
$K_{max} = \hbar\omega - \phi$

ϕ ← WORK FUNCTION

IN MODERN TIMES, THIS EFFECT IS USED TO MAP BAND STRUCTURE

100 YEARS LATER, WE ARE STILL PERFORMING THIS SAME MEASUREMENT TO LEARN ABOUT BAND STRUCTURES IN MATERIALS. THESE DAYS WE ARE CAREFUL ABOUT KEEPING TRACK OF THE ANGLES OF INCOMING PHOTON AND OUTGOING ELECTRON AND REFER TO THE TECHNIQUE AS ANGLE RESOLVED PHOTO ~~EMISSION~~ EMISSION SPECTROSCOPY (ARPES)

ARPES BASIC SETUP



CALL FINAL e^- MOMENTUM (i.e THE ONE MEASURED), $\vec{k}_f$, AND FINAL ENERGY E_{final}

ENERGY IS MEASURED DIRECTLY USING AN ANALYZER BASED PURELY ON ELECTRIC FIELDS AND LORENTZ FORCES, DIRECTION OF $\vec{k}_f$ IS ALSO MEASURED, AND MAGNITUDE IS GIVEN BY $k_f = \sqrt{2m E_{final}}$

WHAT WE WANT TO KNOW IS THE ENERGY AND MOMENTUM (k) OF ELECTRON IN THE SOLID BEFORE THE PHOTON HIT IT BREAKING DOWN INTO COMPONENTS PARALLEL AND PERPENDICULAR TO THE SURFACE

$\hbar k_{e,\parallel} = \hbar k_{s,\parallel} + \hbar k_{\gamma}^{\text{negl}} \approx \sqrt{2m E_F} \sin\theta$

$k_\gamma = \frac{10eV}{E} \sim 0.05 \text{Å}^{-1}$

THE ENERGY OF THE INITIAL ELECTRON IS ALSO FAIRLY STRAIGHTFORWARD, AS IT IS FOUND SIMPLY FROM CONSERVATION OF ENERGY

$$E_{final} = \hbar\omega - E_i - \phi$$

WHERE ϕ IS THE POORLY UNDERSTOOD "WORK FUNCTION" CHARACTERIZING HOW HARD IT IS TO RIP AN ELECTRON FROM THE SOLID SURFACE. IT CAN USUALLY BE GLEANED FROM DATA THOUGH, AS WE WILL SEE.

HARDEST OF ALL TO DETERMINE IS THE COMPONENT OF $\vec{k}_i$ $\perp$ TO THE SURFACE, AS THE ABRUPT CHANGE IN THE POTENTIAL IN THIS DIRECTION MEANS $k_\perp$ IS NOT CONSERVED WHEN THE ELECTRON LEAVES. THERE ARE SEVERAL SCHEMES FOR EXTRACTING THIS INFO, THE MOST COMMON OF WHICH IT TO ASSUME

(1) SCATTERING CAN BE BROKEN DOWN INTO STEPS, FIRST PROMOTING ELECTRONS TO HIGHER BANDS, WHICH THEN ARE FREE TO TRAVEL THROUGH THE METAL SURFACE

THREE STEP MODEL → PROMOTE, TRAVEL, TRANSMIT

AND (2) THESE HIGH ENERGY BANDS ARE FREE ELECTRON LIKE.

IN THIS CASE, ONE CAN SHOW

$$k_\perp = \frac{1}{\hbar}\sqrt{2m\left(E_{final}\cos^2\theta + V_0\right)}$$

WHERE V_0 IS DISTANCE FROM BOTTOM OF VALENCE BAND TO VACUUM

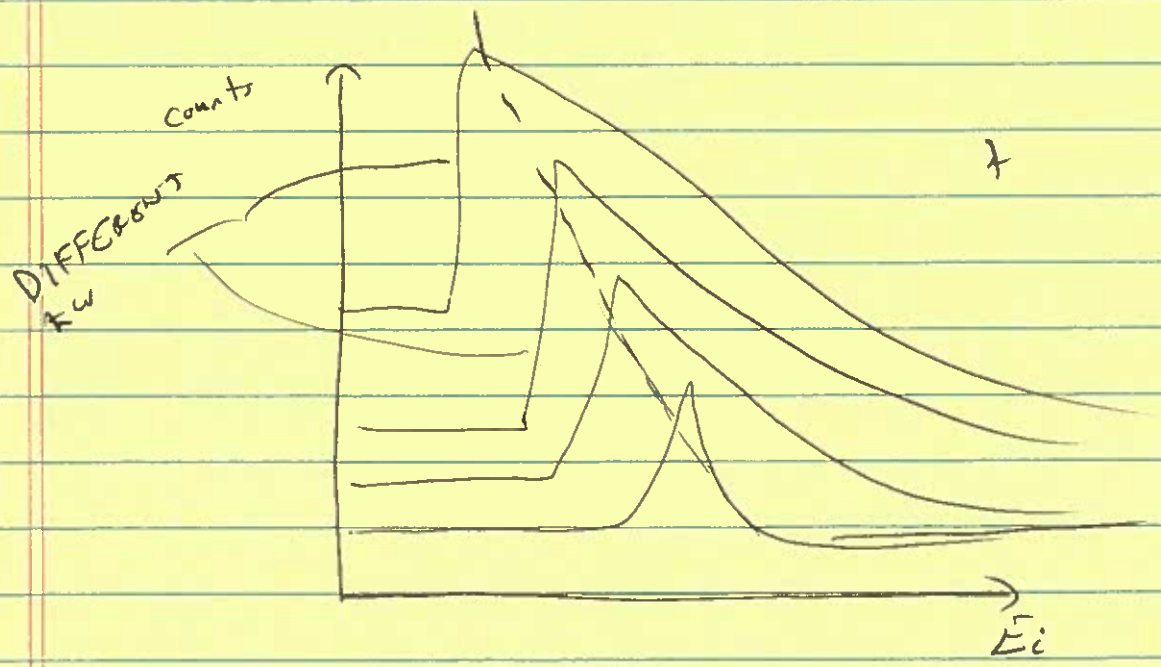
EITHER WAY, WE CAN SEE THAT THERE ARE TWO PIECES OF INFORMATION THAT AN EXPERIMENTALIST CAN USE TO UNIQUELY DETERMINE

K_0 & E_i : E_{final} & $\hbar\omega$

E_{final} GIVES E_i (WITH $\hbar\omega$ GIVEN)

(e.g.) $k_i = \sqrt{2mE_{kin}}$ $\qquad E_i = \hbar\omega - \phi - E_{final}$

TYPICAL DATA LOOKS AS FOLLOWS



VARIATION OF PEAK POSITION (i.e. ELECTRON ENERGY) WITH PHOTON ENERGY (WHICH GIVES k_i) DEFINES DISPERSION RELATIONS. HIGHEST E_i MEASURED GIVES E_{FERMI}

NOTE THAT THIS TECHNIQUE ONLY PROBES OCCUPIED ELECTRON BANDS

IT IS ALSO EXTREMELY SURFACE SENSITIVE WHICH CAN BE A SERIOUS EXPERIMENTAL CONSTRAINT

How else can we measure Fermi surfaces? The tried and true ways is to look for oscillatory behavior in applied magnetic fields. It is worth then stopping to consider this case

Electrons in a uniform magnetic field

Let's adopt momentarily a "semi classical" analysis, where we acknowledge electrons have vectors, $\vec{k}$, and live in bands with energy, $\varepsilon_n(\vec{k})$, but otherwise are treated like classical particles (akin to Sommerfeld theory). In this case, we can write

$$\dot{\vec{p}} = \hbar \dot{\vec{k}} = -\frac{e}{c} \vec{v}_n \times \vec{B} \qquad \text{(Lorentz force law)}$$

($\dot{\vec{p}}$: time derivative)

$$= -\frac{e}{\hbar c} \vec{\nabla}_{\vec{k}} \varepsilon_n \times \vec{B} \qquad \left(\text{Group velocity } v = \frac{\partial \varepsilon}{\partial k}\right)$$

But if we take the dot product of this entire equation with $\vec{\nabla}_{\vec{k}} \varepsilon_n$, we get

$$\hbar \dot{\vec{k}} \cdot \vec{\nabla}_{\vec{k}} \varepsilon_n = 0$$

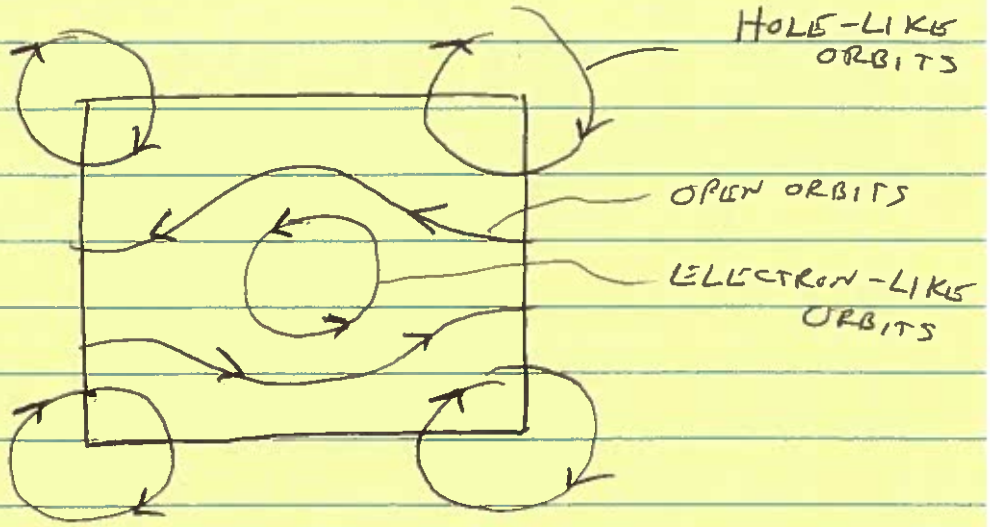
$$\Rightarrow \boxed{\frac{d\varepsilon_n}{dt} = 0}$$

Also

$$\dot{\vec{k}} \cdot \vec{B} = 0 \quad \Rightarrow \boxed{\frac{d(\vec{k} \cdot \vec{B})}{dt} = 0}$$

That is, electrons move in planes perpendicular to the applied field along contours of constant $\varepsilon_n(\vec{k})$

FOR EXAMPLE, IN A 2D BRILLOUIN ZONE, WE MAY HAVE CONSTANT $\mathcal{E}_n(\vec{k})$ CONTOURS



WHERE DIRECTIONS OF MOTION ARE DETERMINED BY GRADIENT $\vec{\nabla}_{\vec{k}} \mathcal{E}_n$

IT MAY BE DIFFICULT TO INTERPRET THIS MOTION AT FIRST, BUT IF WE NOW TAKE THE CROSS-PRODUCT BETWEEN $\hat{B}$ AND OUR FIRST EQUATION

VECTOR TRIPLE PRODUCT: $\vec{a}\times(\vec{b}\times\vec{c}) = \vec{b}(\vec{a}\cdot\vec{c}) - \vec{c}(\vec{a}\cdot\vec{b})$

$$\hat{B} \times \hbar \dot{\vec{k}} = -\frac{e}{c}\hat{B}\times(\vec{v}_n \times \vec{B})$$

$$= -\frac{eB}{c}\left[\vec{v}_n(\vec{k}) - \hat{B}\left(\hat{B}\cdot\vec{v}_n(\vec{k})\right)\right]$$

$$= -\frac{eB}{c}\,\vec{v}_{n\perp}(\vec{k})$$

IN-PLANE VELOCITY

INTEGRATE THIS EQUATION

$$\Rightarrow \frac{-\hbar c}{eB}\hat{B}\times\left[\vec{k}(t) - \vec{k}(0)\right] = \vec{r}_\perp(t) - \vec{r}_\perp(0)$$

i.e. MOTION IN REAL SPACE IS JUST SCALED AND ROTATED VERSION OF k-SPACE MOTION

FOR THIS REASON, ON CALLS ORBITALS WHERE ELECTRONS TRAVEL CCW "ELECTRON-LIKE", BECAUSE THAT IS ALSO HOW A FREE ELECTRON MOVES. PATHS WITH CW MOTION APPEAR TO HAVE OPPOSITE CHARGE, AND ARE CALLED "HOLE-LIKE". THESE ORBITALS ALWAYS STRADDLE BZ BOUNDARIES. AT INTERMEDIATES VALUES OF $\vec{k}$, WE CAN ALSO HAVE "OPEN ORBITALS.

FOR CLOSED ORBITS, WE CAN FURTHER RELATE THE ORBITAL PERIOD TO THE BAND STRUCTURE. FOR SIMPLICITY CONSIDER A NEAR PARABOLIC BAND, WHICH WE SAW WAS A GOOD APPROXIMATION NEAR ZONE CENTERS AND EDGES

GENERALLY $$T = \int_{t_1}^{t_2} dt = \oint \frac{dk}{|\dot{\vec{k}}|} = \oint \frac{dk}{|(\vec{\nabla}_k \varepsilon_n)_\perp|} \frac{\hbar^2 c}{eB}$$

AGAIN, FROM FIRST EQUATION

FOR $\varepsilon = \frac{\hbar^2 k^2}{2m^*} \Rightarrow \vec{\nabla}_{\vec{k}} \varepsilon = \frac{\hbar^2}{m^*}\left(k_x \hat{x} + k_y \hat{y}\right)$

$$|\vec{\nabla}_{\vec{k}} \varepsilon| = \frac{\hbar^2}{m^*}\left(k_x^2 + k_y^2\right)^{\frac{1}{2}} = \frac{\hbar^2 k}{m^*}$$

$$\Rightarrow T = \frac{\hbar^2 c}{eB} \times \frac{m^*}{\hbar^2} \oint \frac{d\vec{k}}{k} = \frac{m^* c}{eB} \int_0^{2\pi} d\phi$$

$$= \frac{2\pi}{\left(\frac{eB}{m^* c}\right)}$$

WHICH ALLOWS US TO DEFINE CYCLOTRON FREQUENCY

$$\omega_c \equiv \frac{eB}{m^* c}$$

WHICH AGAIN CONTAINS EFFECTIVE MASS,

IN MORE GENERAL CASES, IT IS POSSIBLE TO SHOW THAT

$$T = \frac{\hbar^2 c}{eB} \left| \frac{\partial A}{\partial \mathcal{E}} \right|$$

WHERE A IS THE AREA IN k-SPACE OF AN ORBITAL WITH ENERGY $\mathcal{E}$

QUANTUM MECHANIC SOLUTION

IF WE PERFORM THE FULL QUANTUM CALCULATION, WE AGAIN SEE CYCLOTRON FREQUENCY (AND MORE GENERAL ORBITAL SHAPES) CROP UP.

AGAIN, LOOK AT FREE ELECTRON CASE WITH $\vec{B} = B\hat{z}$. FOR QUANTUM CALCULATIONS, IT IS BETTER TO FIND AN APPROPRIATE VECTOR POTENTIAL $\vec{A}$, SUCH THAT

$$\vec{B} = \vec{\nabla} \times \vec{A}$$

THEN, THE HAMILTONIAN WILL BE

$$\mathcal{H} = \frac{1}{2m^*}\left(\vec{p} + \frac{e}{c}\vec{A}\right)^2$$

THIS PROBLEM WAS FAMOUSLY SOLVED BY, AGAIN, LEV LANDAU. FOLLOWING HIS CONVENTION, CHOOSE

$$\vec{A} = Bx\,\hat{y} \qquad \text{- LANDAU GAUGE}$$

$$\rightarrow \quad \hat{H} = \frac{\hat{p}_x^2}{2m^*} + \frac{1}{2m^*}\left(\hat{p}_y + \frac{eB\hat{x}}{c}\right)^2$$

SINCE THE HAMILTONIAN [redacted] COMMUTES WITH $\hat{p}_y$, THE SOLUTION WILL HAVE FORM

$$\psi_k = e^{iky}\,\phi_k(x) \qquad (\text{FREE IN } \hat{y})$$

PLUG INTO SCHRODINGER EQUATION GIVES

$$\left[\frac{\hat{p}_x^2}{2m^*} + \frac{1}{2m^*}\left(\hbar k + \frac{eB\hat{x}}{c}\right)^2\right]\phi_k(x) = E_k\,\phi_k(x)$$

$$\left[\frac{\hat{p}_x^2}{2m^*} + \frac{m^*}{2}\left(\frac{eB}{m^*c}\right)^2\left(\hat{x} + k\frac{\hbar c}{eB}\right)^2\right]\phi_k = E_k\phi_k$$

(ω_c! $\quad$ ℓ^2 $\quad$ 1D)

BOT THIS IS JUST THE "HARMONIC OSCILLATOR" EQUATION IN $\hat{x}$, OFFSET BY AN AMOUNT $\frac{k\hbar c}{eB}$

SOLUTIONS HAVE

$$E_{nk} = \left(n + \tfrac{1}{2}\right)\hbar\omega_c \quad , \; n \in \mathbb{N}$$

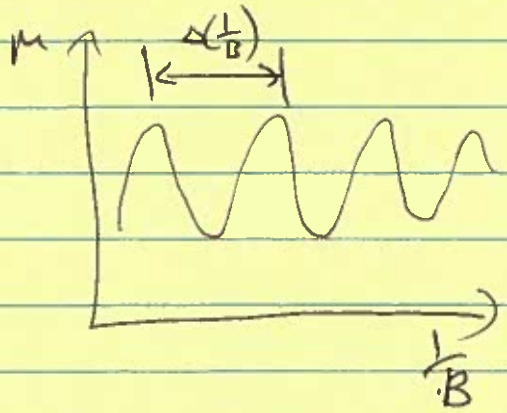
{ LANDAU LEVELS

$$\psi_{nk} = \frac{1}{\sqrt{L}}\,e^{iky}\,H_n\left(x + k\ell^2\right)e^{-\frac{(x+k\ell^2)^2}{2\ell^2}}$$

THE QUANTUM STATES, n, ARE REFERRED TO AS "LANDAU LEVELS" AND CAN BE MOVED IN ENERGY BY CHANGING THE STRENGTH OF THE FIELD.

THIS FACT CREATES A VARIETY OF OSCILLATORY BEHAVIORS AS $E_n \propto \frac{1}{B}$ CROSSES THE FERMI ENERGY. THE MOST FAMOUS OF THESE EFFECTS IS THE VARIATION IN MEASURED MAGNETIZATION WITH FIELD, KNOWN AS THE DE-HAAS - VAN ALPHEN EFFECT, AND I PRESENT WITHOUT PROOF THAT THE VARIATION CAN BE DESCRIBED BY THE EQUATION

$$\Delta\left(\frac{1}{B}\right) = \frac{2\pi e}{\hbar A_c}$$



WHERE A_c IS THE AREA OF EXTEMAL ORBITS IN THE PLAN $\perp \vec{B}$

ANALOGOUS BEHAVIOUR IS OBSERVED IN MEASUREMENTS OF RESISTIVITY, THERMAL TRANSPORT, ULTRASONIC ATTENUATION, AND MANY OTHERS AT LOW TEMPERATURES AND HIGH FIELDS

$$k_B T \ll \hbar\omega_c$$