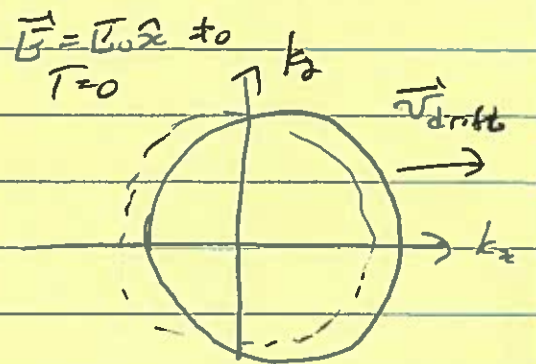
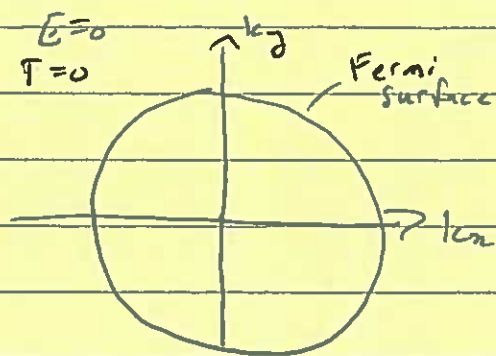


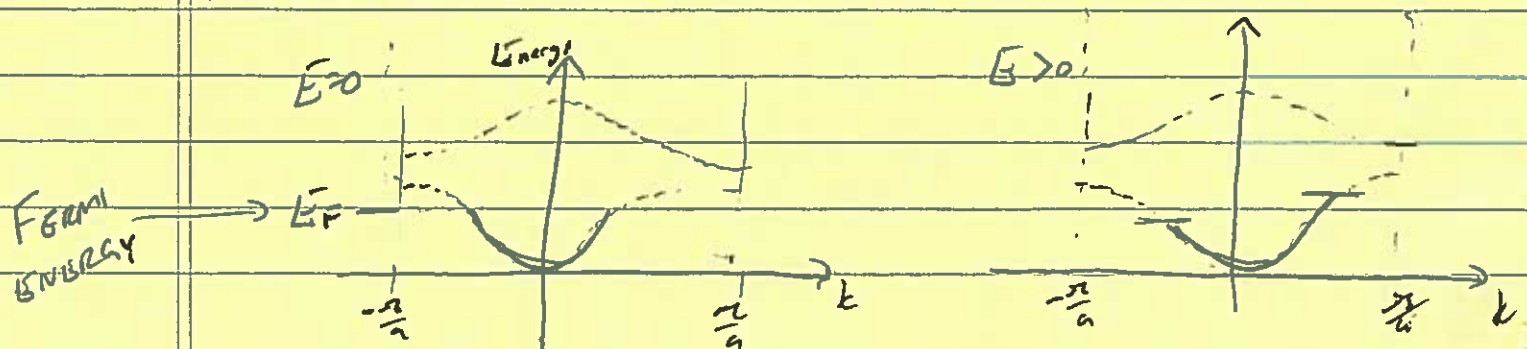
PHYS 460 - LECTURE 12

NOW THAT WE HAVE SPENT SOME TIME EXPLORING THE BEHAVIOR OF ELECTRONS IN A PERIODIC POTENTIAL, IT IS WORTH REVISITING THE QUESTION OF WHETHER A ~~METAL~~ MATERIAL IS A METAL OR AN INSULATOR, AND HOW TO PREDICT WHICH A MATERIAL WILL BE

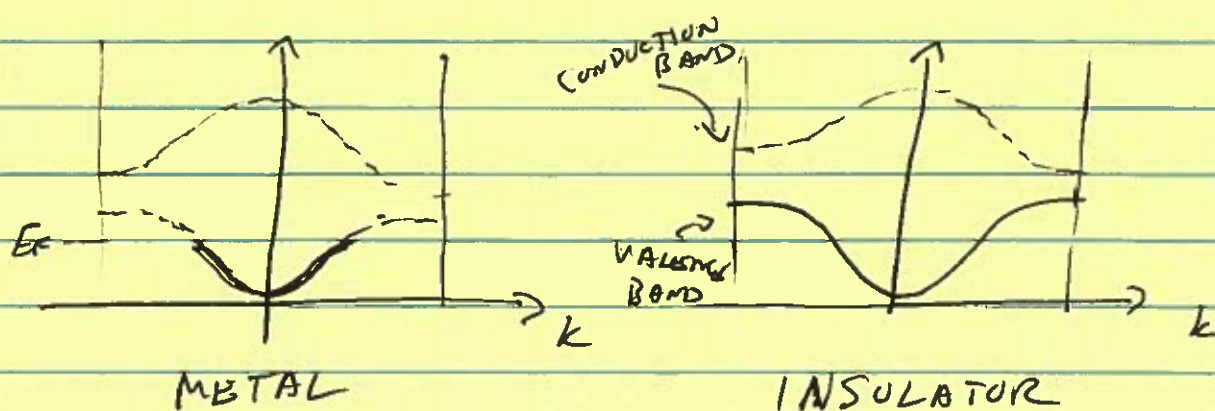
FIRST LET'S RECALL WHAT IT MEANS TO BE A METAL. A "METAL", WE SAY, IS A MATERIAL WHICH WILL CARRY ELECTRICAL CURRENT IF WE APPLY AN INFINITESIMAL ELECTRIC POTENTIAL DIFFERENT. IN TERMS OF QUANTUM MECHANICS, THIS MEANS THAT AN ELECTRIC FIELD HAS THE ABILITY TO SELECTIVELY SHIFT OCCUPATION OF k -STATES TOWARD THE DIRECTION OF THE FIELD. IN 2D, I PREVIOUSLY DRAW



SIMON SHOWS A SIMILAR PLOT IN 1D, WHICH PERHAPS IS EVEN CLEARER



IN BOTH SETS OF PLOTS, IT IS CLEAR THAT BY INCREASING "RIGHTMOST" k -STATES MORE FAVORABLY, THE FIELD INDUCES A NET DRIFT OF ELECTRONS. IN THE 1D PLOTS, IT BECOMES CLEAR THAT THIS REDISTRIBUTION IS ONLY POSSIBLE IF THERE EXIST OPEN ELECTRON ENERGY LEVELS IMMEDIATELY ABOVE THE HIGHEST ENERGY OCCUPIED STATE



NOTE THAT IN THE CASE OF THE INSULATOR, IT SUDDENLY BECOMES UNCLEAR WHERE TO LABEL $E = E_F$. (THE CONVENTION IS MIDWAY BETWEEN THE BANDS.) THIS OBSERVATION OFTEN LEADS TO AN ALTERNATE (TONGUE-IN-CHEEK) DEFINITION OF A METAL:

"A METAL IS A SOLID WITH //
A FERMI SURFACE"

So How Do We Predict If A Material Is A Metal?

Well, first we note the total number of electrons free to travel per unit cell. Then

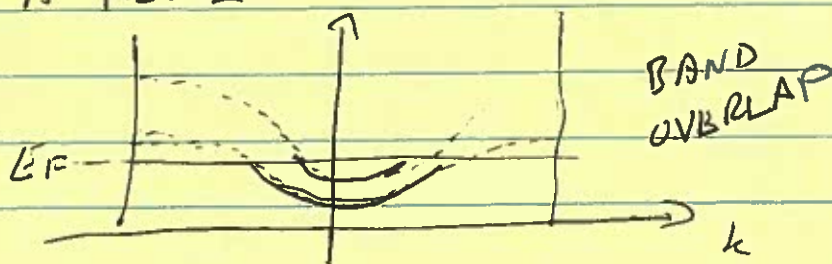
① If there are an odd number of electrons, the material is a metal. Why? Because there are exactly N available k -states in the 1st BZ, but each state can be occupied twice - once for each electron spin orientation

→ odd # electrons always leave a band half filled! e.g. alkali metals

② Having an even number of electrons is a necessary but not sufficient condition for being an insulator

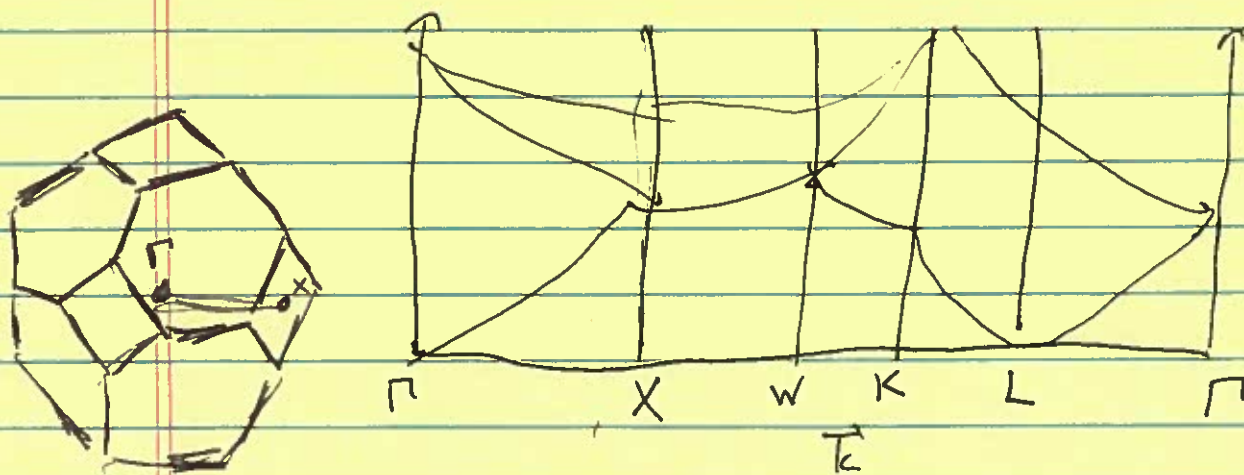
→ If an even number of electrons fully complete a band, the material is a band insulator

③ If the lowest point of any upper band dips below $E = E_F$, one can again create a metal



HOW DOES THIS PICTURE CHANGE IN HIGHER DIMENSIONS? NOT MUCH. THERE IS JUST MORE TO KEEP TRACK OF. IT'S HARD TO PLOT EVERYTHING AT ONCE, AND SO ~~THE~~ CERTAIN CONVENTIONS HAVE COME INTO BEING

ONE IS TO PLOT BANDS ALONG HIGH SYMMETRY DIRECTIONS ONLY IN A 1D PLOT. OFTEN YOU SEE SOMETHING LIKE



ACCOMPANIED BY A PLOT DEFINING THE LOCATIONS IN THE BZ THAT IS MEANT BY THE GREEK LETTERS

CONVENTIONS ARE

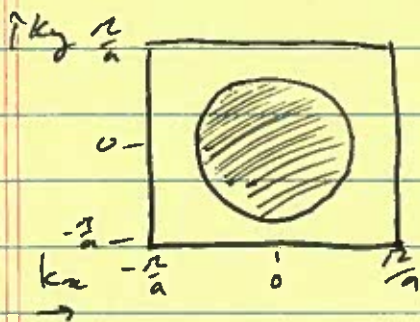
- Γ - CENTER OF ZONE
- M - CENTER OF EDGE
- R - CORNER
- X - CENTER OF FACE

⋮

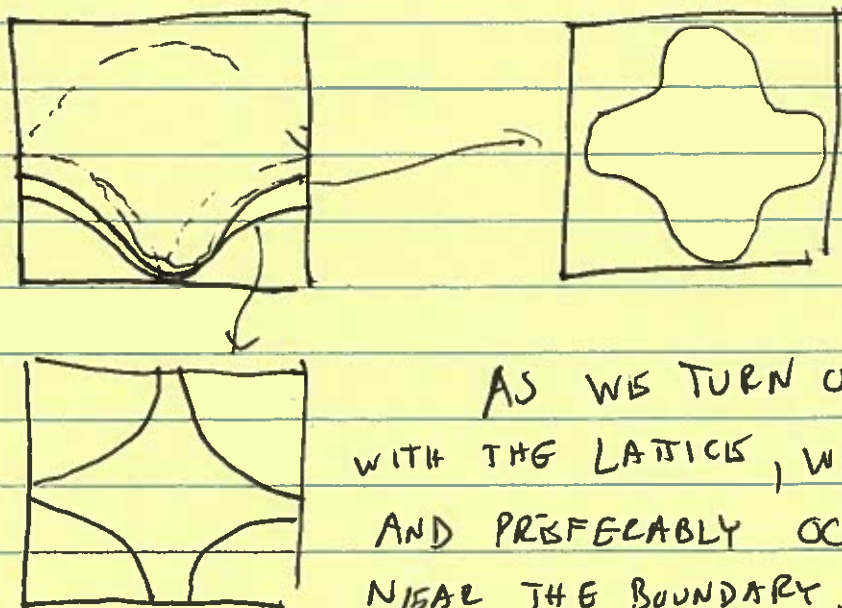
AND SO ON

ANOTHER PLOT OF CENTRAL IMPORTANCE IS THE LOCUS OF POINTS IN k -SPACE WITH CONSTANT ENERGY $E = E_F$. i.e. THE "FERMI SURFACE"

2D FOR EXAMPLE CONSIDER THE CASE OF MONOVALENT IONS ON A SQUARE LATTICE. IF YOU PLOT THE FILLED STATES (AT $T=0$), YOU WILL MAP OUT A PERFECT CIRCLE IN THE FIRST BZ.



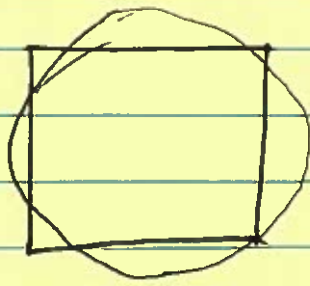
NOTE IN THIS CASE, THE 1ST BZ IS EXACTLY HALF FILLED. THERE ARE ALSO STATES INFINITELY CLOSE IN $E \rightarrow$ METAL (GAPPING IS ALWAYS AT ZONE BOUNDARY)



AS WE TURN ON INTERACTIONS WITH THE LATTICE, WE PUSH DOWN AND PREFERABLY OCCUPY STATES NEAR THE BOUNDARY, WHICH DISTORTS THE FERMI SURFACES WHILE CONSERVING AREA

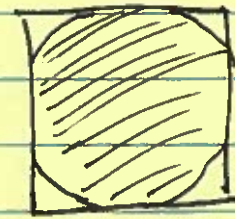
IF INTERACTIONS ARE STRONG ENOUGH, THE SURFACES CAN TOUCH THE ZONE BOUNDARY, BUT THE MATERIAL REMAINS A METAL

NOW WHAT HAPPENS IF WE DOUBLE THE NUMBER OF ELECTRONS. WITHOUT LATTICE INTERACTIONS THE FERMI SURFACE SPILLS INTO THE 2nd (AND 3rd) ZONES



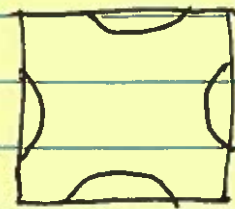
OR IN REDUCED ZONE SCHEMES

1st zone

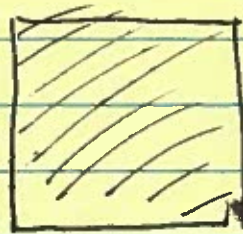


→ CLOSE STATES
⇒ METAL

2nd zone



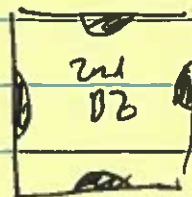
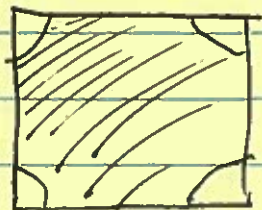
IF WE EXAMINE LARGE INTERACTIONS, THE SYSTEM HAS EXACTLY ENOUGH ELECTRONS TO FILL UP THE 1ST ZONE



AND THE SECOND ZONE
1) GAPPED AT THE BOUNDARY
→ BAND INSULATOR

THERE ARE ALWAYS INTERMEDIATE CASES WHERE THE SPINER IS NOT ~~COMPLETELY~~ STRONG ENOUGH TO COMPLETELY DISTORT THE FERMI SPHERES

1st BZ



"OVERLAPPING BANDS"

→ METAL

IN GENERAL, IF THERE IS A FERMI SURFACE → METAL

FAILURES OF BAND THEORY

YOU MAY HAVE NOTICED THAT I HAVE BEEN REFERRING TO MATERIALS AS "BAND INSULATORS" AND NOT SIMPLY "INSULATORS". WHY IS THAT? WELL, AS YOU MAY HAVE (AND PROBABLY SHOULD HAVE) ANTICIPATED, BAND THEORY DOES NOT ALWAYS WORK.

AS WITH ANY THEORY THIS IS A RESULT OF A BREAK DOWN OF OUR UNDERLYING ASSUMPTIONS. WE HAVE MADE MANY, BUT THE BIGGEST ONE IS THAT WE CAN IGNORE ELECTRON-ELECTRON INTERACTIONS (THE INDEPENDENT ELECTRON PICTURE)!

IF WE JUST CHECK THE ENERGY SCALES OF ELECTRONS USING COULOMB'S LAW THOUGHT, WE FIND

$$\Delta_{e-e} \sim \frac{ke^2}{r} \sim 10\text{eV} \gg \epsilon_F$$

THIS SHOULD NEVER WORK!

THE REASON IT DOES WAS WORKED OUT BY RUSSIAN PHYSICIST LEV LANDAU IN HIS NOW FAMOUS "FERMI-LIQUID THEORY"

THE SPECIFICS ARE TOO COMPLEX TO GO INTO HERE, BUT ~~BASICALLY~~ STATES THAT "IF THE INTERACTING MANY BODY ELECTRONIC STATE IS ADIABATICALLY CONNECTED TO THE INDEPENDENT e^- STATE, THEN THERE IS A ONE-TO-ONE MAPPING BETWEEN ENERGY STATES NEAR THE FERMI SURFACE", BASICALLY SAYING THAT IN CASES WHERE IT WORKS THE CHARGE CARRYING PARTICLES LOOK JUST LIKE ELECTRONS. THE MAIN CAVEAT IS THEY CAN NOW HAVE DIFFERENT m^* , e^* , μ^* etc

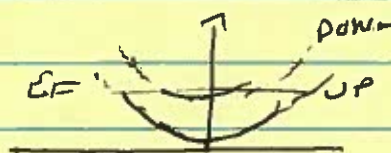
"quasi-particles"
→

SO LEV LANDAU TELLS US IT IS OKAY TO TALK ABOUT METALS IF THE MATERIAL IS CLOSE ENOUGH TO THE METALLIC STATE. WHEN IT IS NOT "CLOSE ENOUGH" THAT USUALLY MEANS SOMETHING DRAMATIC HAS HAPPENED

A COUPLE OF FAILURES ALONG THIS LINE

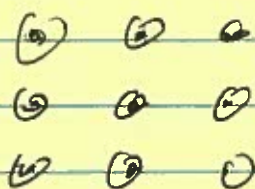
- ① MAGNETISM - SO FAR WE HAVE BEEN NEGLECTING ELECTRON SPIN, EXCEPT WHEN WE ARE COUNTING DEGREES OF FREEDOM. WE WILL FIND CASES HOWEVER WHEN ONE (E.G. "SPIN UP") BAND IS LOWER IN ENERGY THAN THE OTHER ("SPIN DOWN")

→ MAGNETIC STATE



THIS AND MORE COMPLEX STATES
CONSIDERED LATER

- ② MOTT INSULATOR - IN CASES OF VERY STRONG e^-e^- INTERACTIONS, ELECTRONS DON'T LIKE TO BE NEAR EACH OTHER AT ALL, AND THEY LOCALIZE TO MAINTAIN MAXIMUM AVOIDANCE. IN THIS WAY, EVEN HALF FILLED BANDS (WHICH SHOULD BE METALS) CAN BE STRONG INSULATORS. → "MOTT INSULATOR"



THIS IS AN IMPORTANT
BUT VERY DIFFICULT
PROBLEM IN MODERN PHYSICS
e.g. NiO , La_2CuO_4

③ SUPERCONDUCTIVITY - NORMALLY REPULSIVE, IN 1957 BARDEEN AND STUDENTS AT UIUC SHOWED THAT IF THERE WAS ANY WAY TO FORM AN ATTRACTIVE INTERACTION BETWEEN ELECTRONS, THEN THEY WOULD "PAIR UP" (COOPER PAIRS) TO EFFECTIVELY FORM BOSONS AND THE ENTIRE FERMI SURFACE WOULD COLLAPSE.

THE RESULTING GROUND STATE WOULD BE A QUANTUM MECHANICAL MANY-BODY WAVE FUNCTION ABLE TO CARRY CURRENTS WITHOUT RESISTANCE AND EXCEL MAGNET FIELDS
→ SUPERCONDUCTIVITY

AGAIN, WE WILL LIKELY REVIEW THIS TOPIC AT A LATER TIME.

OK, SO WHAT IS A SEMICONDUCTOR?

THIS IS A "FALSE" CLASS OF MATERIALS IN THAT, AT $T=0K$, SEMICONDUCTORS ARE INSULATORS

HOWEVER THE BAND GAP IS SMALL ENOUGH THAT AT ROOM TEMPERATURE, A SMALL AMOUNT OF CHARGE CARRIERS ARE THERMALLY EXCITED ACROSS THE GAP TO THE CONDUCTION BAND AND CAN CARRY CURRENT. IT TURNS OUT THAT SUCH MATERIALS ARE WELL SUITED TO BAND ENGINEERING AND FORM THE BASIS OF MUCH OF MODERN TECH.

