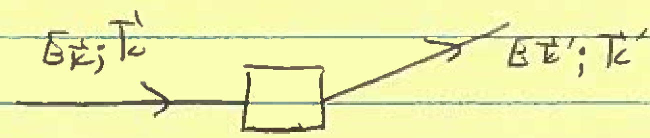
PHYS 460 LECTURE 9

WE ARE NOW IN A POSITION TO TALK ABOUT ELECTRONS INSIDE A PERIODIC POTENTIAL. BEFORE WE DIVE IN HOWEVER, IT IS WORTH BRIEFLY REVIEWING THE LAST THING WE TALKED ABOUT

INELASTIC NEUTRON SCATTERING



ONE CAN DERIVE THE SCATTERING CONDITIONS FROM FERMI'S GOLDEN RULE (PERTURBATION THEORY) OR BRAGG'S LAW, IN THE CASE OF DIFFRACTION, BUT ONE FINDS THAT SCATTERING SIMPLY OBEYS TWO CONSERVATION EQUATIONS:

$$① \quad E_{\vec{k}'} - E_{\vec{k}} = -\sum_{\vec{p}} \hbar\omega_{\vec{p}} \Delta n_{\vec{p}}$$

WHERE $\Delta n_{\vec{p}}$ IS THE CHANGE IN OCCUPANCY OF PHONON MODE $\vec{p}$

AND

$$② \quad \hbar\vec{k}' - \hbar\vec{k} = -\sum_{\vec{p}} \hbar\vec{p}\,\Delta n_{\vec{p}} + \hbar\vec{G}$$

THE FIRST RULE IS SIMPLY CONSERVATION OF ENERGY, AND STATES THAT ANY CHANGE IN THE KINETIC ENERGY OF THE NEUTRON MUST BE COMPENSATED FOR ~~B~~ BY THE CREATION OR ANNIHILATION OF PHONONS. THE SECOND EQUATION ~~~~ COMES DIRECTLY FROM THE DISCRETE TRANSLATIONAL SYMMETRY OF THE

CRYSTAL, AND BE INTERPRETED AS A CONSERVATION OF "CRYSTAL MOMENTUM". THAT IS, THE CHANGE IN NEUTRON MOMENTUM IS COMPENSATED FOR BY THE MOMENTUM OF PHONONS CREATED/DESTROYED TO WITHIN AN ADDITIVE FACTOR OF RECIPROCAL LATTICE VECTOR, $\vec{G}$.

ANY NUMBER OF PHONONS CAN BE CREATED IN THESE SCATTERING EVENTS, BUT ONE USUALLY RESTRICTS ATTENTION TO A FEW SPECIAL CASES:

I ZERO PHONON SCATTERING $(\Delta n_{\vec{p}} = 0 \ \forall \vec{p})$

$$\Rightarrow \quad E_{\vec{k}'} = E_{\vec{k}} \quad \text{AND} \quad \vec{k}' - \vec{k} = \vec{G}$$

$\longrightarrow$ LAUE CONDITION!

WE NOW SEE THAT THE LAUE CONDITION CAN SIMPLY BE RESTATED AS A CONSERVATION OF CRYSTAL MOMENTUM

II ONE PHONON SCATTERING $(\Delta n_{\vec{p}} = 1)$

A SINGLE PHONON IS EXCITED/DESTROYED BY THE NEUTRON. IF IT HAS "MOMENTUM", $\vec{p}$

e.g. ABSORPTION EVENT

$$E_{\vec{k}'} = E_{\vec{k}} + \hbar\omega_{\vec{p}}$$

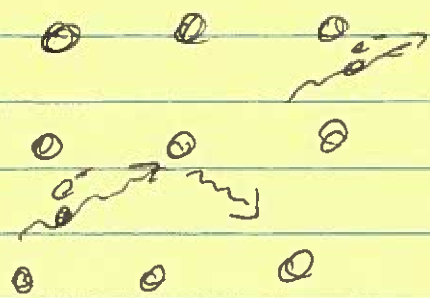
$$\vec{k}' - \vec{k} = \hbar\vec{p} + \hbar\vec{G} \quad \leftarrow \text{CONSERVATION OF CRYSTAL MOMENTUM}$$

FOR DEFINED $\vec{k}$, THIS UNIQUELY DETERMINES $\vec{k}'$

$$\boxed{\frac{\hbar^2|\vec{k}'|^2}{2m_n} - \frac{\hbar^2|\vec{k}|^2}{2m} = \hbar\,\omega(\vec{k}' - \vec{k})}$$

TAKE HOME POINT: CONSERVATION OF ~~CRYSTAL MOM~~ DEFINES ALL SCATTERING EVENTS!

NOW LET'S TURN OUR ATTENTION BACK TO ELECTRONS. WE STARTED THIS COURSE WITH A DISCUSSION OF <u>METALS</u>, AND FOUND THAT WE COULD REPRODUCE MANY OF THEIR PROPERTIES BY TREATING METALS AS GASES OF FREE AND INDEPENDENT ELECTRONS



DRUDE

+ QM → SOMMERFELD

<u>SUCCESSES</u>: EXPLAINED OHM'S LAW, HALL EFFECT, PLASMA FREQUENCY, $C_V \propto \gamma T$, K, ...

AMAZING

BUT THERE WERE <u>SEVERAL</u> NOTABLE FAILURES. SOME ARE FUNDAMENTAL TO THE PICTURE. SPECIFICALLY, WE DON'T KNOW

(1) WHY ISN'T EVERYTHING A METAL?

NB $\left.\begin{array}{l}\rho_{\text{insulators}} \sim 10^{22}\ \Omega\text{-cm} \\ \rho_{\text{metals}} \sim 10^{-10}\ \Omega\text{-cm}\end{array}\right\}$ 10^{32} DIFFERENCE

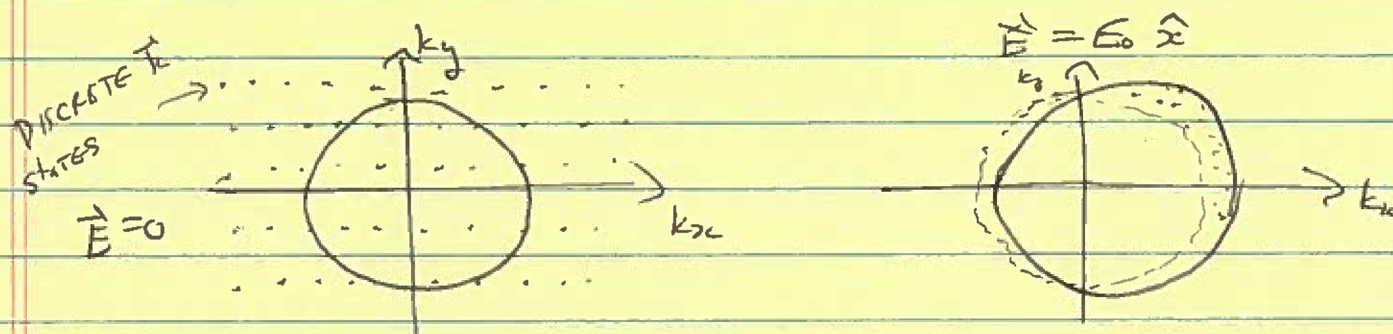
(2) WHAT IS SCATTERING ELECTRONS AND HOW DO THEY AVOID ATOMIC NUCLEI GIVEN KNOWN MEAN FREE PATHS $\ell \sim 1 - 10^{8}$ Å ?

(3) WHY IS R_H POSITIVE SOMETIMES? POSITIVE CHARGE?

OF THESE FAILURES, NUMBER 1 MAY SEEM SIMPLEST, BUT IS THE MOST FUNDAMENTAL. A 32 ORDER OF MAGNITUDE DIFFERENCE IN ρ IS NOT SIMPLY DRUDE THEORY WITH HIGHER SCATTERING RATE. THE MODEL FAILS. INSULATORS ARE FUNDAMENTALLY DIFFERENT BEASTS. HOW AND WHY?

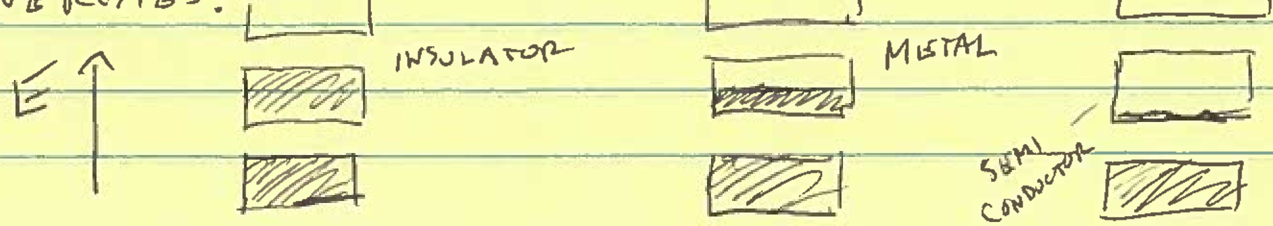
AS YOU MAY HAVE ANTICIPATED, THE ANSWER TO THESE QUESTIONS INVOLVES THE INTERACTION BETWEEN ELECTRONS IN THE MATERIAL AND THE PERIODIC ARRAY OF NUCLEI WHICH, WE WILL SEE, CREATES SO-CALLED "GAPS" IN THE ENERGY SPECTRUM OF ELECTRONS.

CONSIDER A FREE ELECTRON FERMI SPHERE



IN QUANTUM SYSTEMS, THERE IS NO SMOOTH ACCELERATION OF PARTICLES. THE CREATION OF A NET ELECTRON VELOCITY INVOLVES THE MOVEMENTS OF SEVERAL PARTLES FROM $\vec{k} \to \vec{k} + dk\hat{x}$ BY FIELD, BUT THIS INVOLVES THAT STATES $\vec{k} + dk\hat{x}$ EXIST!

THIS IS WHERE GAPS COME IN. WE WILL SEE LATTICE INTERACTIONS CREATE DISALLOWED WAVE-VECTORS, $\vec{k}$, OR EQUIVALENTLY GAPS IN THE POSSIBLE ELECTRON ENERGIES.



SO THE QUESTION TRANSFORMS INTO ONE ABOUT THE ORIGIN OF THE GAPS. AS I MENTIONED, THE ORIGIN IS ELECTRON-LATTICE INTERACTIONS, AS ONE CAN SEE IMMEDIATELY, WITH ANY ATTEMPT AT ADDRESSING THE PROBLEM. THE FULL SOLUTION TO THE PERIODIC POTENTIAL HAMILTONIAN (WHICH WE WILL EVENTUALLY TACKLE) IS QUITE COMPLEX. LET'S START SIMPLER

THE "NEARLY" FREE ELECTRON MODEL

THIS IS A COMMON FIRST ATTEMPT AT ADDRESSING ELECTRON-LATTICE INTERACTIONS, AND SAYS THAT AS A FIRST APPROXIMATION, WE CAN USE THE FREE ELECTRON WAVEFUNCTIONS AND APPLY PERTURBATION THEORY

IN THIS SITUATION, WE CAN TREAT ELECTRONS SIMPLY AS WAVES $\psi_k = \psi_0 e^{-i(\omega t - \vec{k}\cdot\vec{r})}$. TO START. BUT WHAT DO WE KNOW ABOUT WAVES INTERACTING WITH A PERIODIC POTENTIAL? THEY <u>SCATTER!</u>

eg 1D LATTICE POTENTIAL

- LAUE CONDITION IN <u>1D</u>

$$k' = k + G$$

$$|k'| = |G| \pm |k|$$

BUT IF $|k'| = |k|$ $\Rightarrow$ $k = \pm\frac{1}{2}G = \pm n\pi a$ $\rightarrow$ BZ ZONE BOUNDARY

SO JUST ANTICIPATING THE FULL SOLUTION FOR A MOMENT, WE KNOW (DEGENERATE) PERTURBATION THEORY IS GOING TO MIX THE k & k' WAVEFUNCTIONS. AT THE EDGES OF THE 1st BZ, ELECTRON ψ_k HAVE THE SAME ENERGY $E_{k'} = E_k = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2 n^2 \pi^2}{2a^2}$

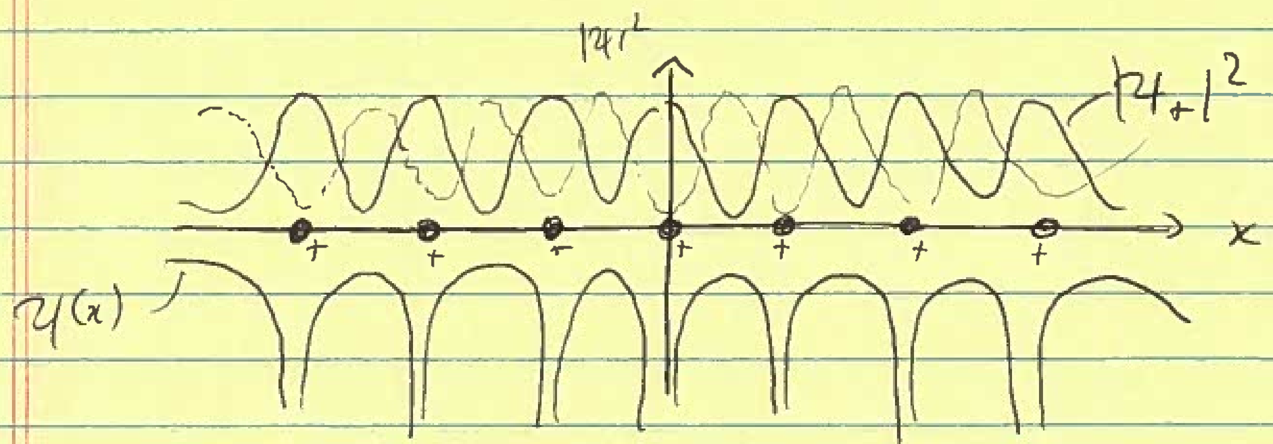
$\rightarrow$ SOLUTIONS WILL BE

$$\psi_+ = \psi_0 e^{\frac{i\pi x}{a}} + \psi_0 e^{-\frac{i\pi x}{a}} = 2\cos\left(\frac{\pi x}{a}\right)$$

AND

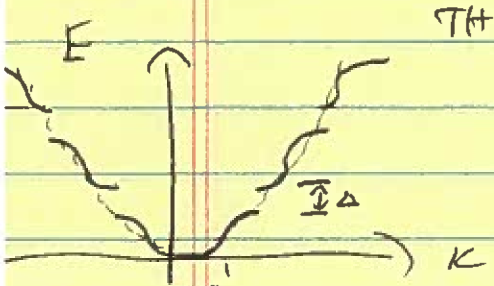
$$\psi_- = \psi_0 e^{\frac{i\pi x}{a}} - \psi_0 e^{-\frac{i\pi x}{a}} = 2i\sin\left(\frac{\pi x}{a}\right)$$

AND THE RESULTANT ELECTRON DENSITY $\rho = |\psi|^2$ FOR THE TWO STATES LOOKS LIKE



THUS THE ψ_+ SOLUTION HAS ELECTRONS ON TOP OF LATTICE POINTS AND MAXIMIZING COLOUMB ENERGY WHILE ψ_- HAS ELECTRONS BETWEEN NUCLEI

THIS LEADS TO A GAP



$$\Delta = \int_0^a dx\, U(x) \left[|\psi_+|^2 - |\psi_-|^2 \right]$$

FOR EXAMPLE

$$= 2\int_0^a dx\, U_0 \cos\left(\frac{2\pi x}{a}\right)\left(\cos^2 - \sin^2\right)$$

$$= \int dx\, U_0 \cos^2\left(\frac{2\pi x}{a}\right) = U \rightarrow \text{FOURIER COMPONENT OF } U(x)$$

OK, LET'S DO THIS PROPERLY. SAY WE HAVE ELECTRONS WHOSE BEHAVIOUR IS DICTATED BY THE HAMILTONIAN

$$\mathcal{H} = K + V(\vec{r})$$

WHERE $K = \frac{p^2}{2m}$ AND $V(\vec{r}) = V(\vec{r} + \vec{R})$

LET $|\vec{k}\rangle$ BE THE SOLUTION TO

$$K|\vec{k}\rangle = \varepsilon_0(\vec{k})\,|\vec{k}\rangle$$

AND $\varepsilon_0(\vec{k}) = \dfrac{\hbar^2 k^2}{2m}$

FROM OUR PREVIOUS EXPERIENCE WITH SCATTERING, WE CAN ALSO SAY THE MATRIX ELEMENTS

$$\langle \vec{k}' | V(\vec{r}) | \vec{k} \rangle = \frac{1}{L^3} \int d\vec{r}\; e^{i(\vec{k}-\vec{k}')\cdot\vec{r}}\, V(\vec{r})$$

$$\equiv V_{\vec{k}'-\vec{k}}$$

$$= 0 \quad \text{UNLESS } \vec{k}' - \vec{k} = \vec{G}$$

LAUE CONDITION AGAIN

NOW, ASSUMING $V \ll \varepsilon_0$, WE START APPLYING PERTURBATION THEORY

<u>1st ORDER</u> $\quad \varepsilon(\vec{k}) = \varepsilon_0(\vec{k}) + \langle \vec{k} | V | \vec{k} \rangle = \varepsilon_0(\vec{k}) + V_0$

→ CONSTANT OFFSET SINCE $\vec{k}' - \vec{k} = 0$

→ NO PHYSICAL CONSEQUENCE

2ND ORDER $$\mathcal{E}(\vec{k}) = \mathcal{E}_0(\vec{k}) + \sum_{\substack{\vec{k}'=\vec{k}+\vec{G} \\ (\vec{G}\neq 0)}} \frac{|\langle \vec{k}'|V|\vec{k}\rangle|^2}{\mathcal{E}_0(\vec{k}) - \mathcal{E}_0(\vec{k}')}$$

IN THE CASE OF DEGENERATE MODES, WHERE $\mathcal{E}_0(\vec{k}') = \mathcal{E}_0(\vec{k})$, IT IS NOT SIMPLY ENOUGH TO SUM OVER FREE ELECTRON STATES $|\vec{k}\rangle$. ONE MUST START BY FINDING NEW WAVEFUNCTIONS

$$|\psi\rangle = \alpha\,|\vec{k}\rangle + \beta\,|\vec{k}'\rangle$$

WHICH DIAGONALIZE THE HAMILTONIAN, $\mathcal{H}$

DEFINING $|\vec{k}'\rangle = |\vec{k}+\vec{G}\rangle$ AND LETTING $V_0 = 0$

$$\langle \vec{k}|\mathcal{H}|\vec{k}\rangle = \mathcal{E}_0(\vec{k})$$
$$\langle \vec{k}'|\mathcal{H}|\vec{k}'\rangle = \mathcal{E}_0(\vec{k}') = \mathcal{E}_0(\vec{k}+\vec{G})$$
$$\langle \vec{k}'|\mathcal{H}|\vec{k}\rangle = \mathcal{E}_0(\vec{k})\langle \vec{k}'|\vec{k}\rangle + V_{\vec{k}'-\vec{k}} = V_{\vec{G}}$$
$$\langle \vec{k}|\mathcal{H}|\vec{k}'\rangle = V_{-\vec{G}} = V_{\vec{G}}^*$$

SINCE $V_{-\vec{G}} = V_{\vec{G}}^*$ IF $V(\vec{r})$ REAL

THUS $\mathcal{H}|\psi\rangle = E|\psi\rangle$ LEADS TO

$$\begin{pmatrix} \mathcal{E}_0(\vec{k}) & V_{\vec{G}}^* \\ V_{\vec{G}} & \mathcal{E}_0(\vec{k}+\vec{G}) \end{pmatrix}\begin{pmatrix}\alpha \\ \beta\end{pmatrix} = E\begin{pmatrix}\alpha \\ \beta\end{pmatrix}$$

$$\Rightarrow \boxed{\left(\mathcal{E}_0(\vec{k}) - E\right)\left(\mathcal{E}_0(\vec{k}+\vec{G}) - E\right) - |V_{\vec{G}}|^2 = 0}$$

CASE 1 : $\vec{k}$ EXACTLY AT BZ BOUNDARY

$\rightarrow \vec{k}' = \vec{k} + \vec{G}$ ALSO AT BZ BOUNDARY

FOR 1ST BZ $\quad \varepsilon_0(\vec{k}) = \varepsilon_0(\vec{k} + \vec{G})$

$$\Rightarrow \quad \left(\varepsilon_0(\vec{k}) - E\right)^2 = |V_{\vec{G}}|^2$$

$$E_\pm = \varepsilon_0(\vec{k}) \pm |V_{\vec{G}}|$$

THUS GAP IS JUST FOURIER COMPONENT OF POTENTIAL $V(\vec{r})$, AS WE HAVE ALREADY SEEN AND OUR MATRIX EQUATION BECOMES

$$\begin{pmatrix} \varepsilon_0 - \varepsilon_0 \mp |V_{\vec{G}}| & V_{\vec{G}}^* \\ V_{\vec{G}} & \varepsilon_0 - \varepsilon_0 \mp |V_{\vec{G}}| \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = 0$$

$$\alpha = \pm \beta$$

ie $\quad |\psi\rangle = \frac{1}{\sqrt{2}}\left(|\vec{k}\rangle \pm |\vec{k}'\rangle\right)$

WHICH FOR OUR 1D CHAIN BECOMES

$$\psi_\pm \propto e^{i\frac{\pi x}{a}} \pm e^{-\frac{\pi x}{a}} = \begin{cases} \cos\left(\frac{\pi x}{a}\right) \\ \sin\left(\frac{\pi x}{a}\right) \end{cases}$$

OUR ASSUMED SOLUTIONS FROM BEFORE

CASE 2: NOW WHAT IF WE MOVED SLIGHTLY AWAY FROM THE BZ BOUNDARY? LET'S STAY IN 1D, AND CONSIDER

$$k = \frac{n\pi}{a} + \delta \qquad \delta \ll \frac{\pi}{a}$$
$$k' = -\frac{n\pi}{a} + \delta$$

PLUG INTO $E_k = \frac{\hbar^2 k^2}{2m}$

$$\varepsilon_0(k) \to \frac{\hbar^2}{2m}\left(\left(\frac{n\pi}{a}\right)^2 + \delta^2 + \frac{2n\pi\delta}{a}\right)$$
$$\varepsilon_0(k') \to \frac{\hbar^2}{2m}\left(\left(\frac{n\pi}{a}\right)^2 + \delta - \frac{2n\pi\delta}{a}\right)$$

AND OUR EIGENVALUE EQUATION BECOMES

$$\left(\frac{\hbar^2}{2m}\left[\left(\frac{n\pi}{a}\right)^2 + \delta^2\right] + \frac{\hbar^2}{2m}\cdot\frac{2n\pi\delta}{a} - E\right)$$
$$\times\left(\frac{\hbar^2}{2m}\left[\left(\frac{n\pi^2}{a}\right) + \delta^2\right] - \frac{\hbar^2}{2m}\cdot\frac{2n\pi\delta}{a} - E\right) = |V_G|^2$$

DIFFERENCE OF SQUARES FORMULA

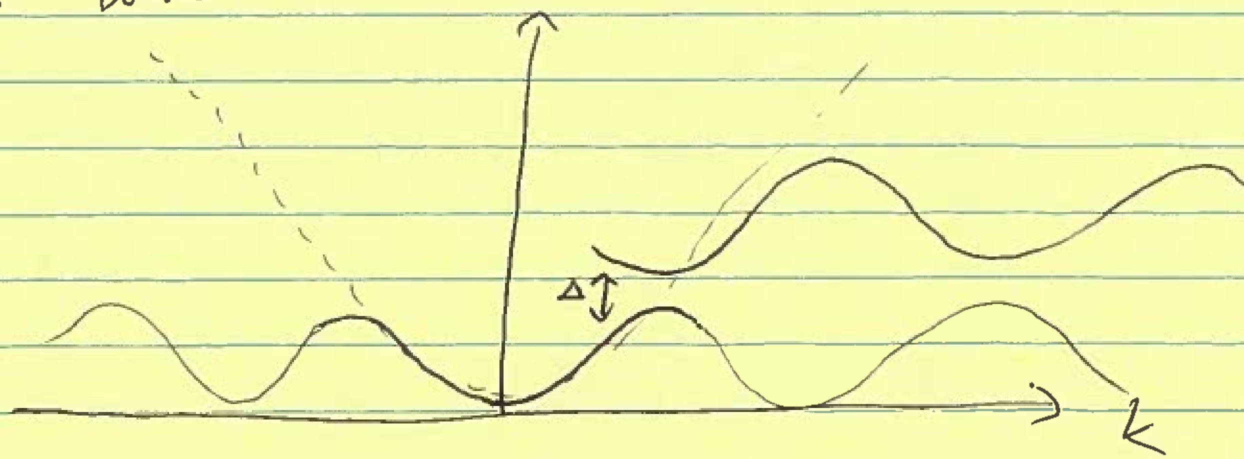
$$\to \left(\frac{\hbar^2}{2m}\left[\left(\frac{n\pi}{a}\right)^2 + \delta^2\right] - E\right)^2 - \left(\frac{\hbar^2}{2m}\frac{2n\pi\delta}{a}\right)^2 = |V_G|^2$$

$$E_\pm = \frac{\hbar^2}{2m}\left[\left(\frac{n\pi}{a}\right)^2 + \delta^2\right] \pm \sqrt{\left(\frac{\hbar^2}{2m}\frac{2\pi n\delta}{a}\right)^2 + |V_G|^2}$$

$$= \frac{\hbar^2}{2m}\left[\left(\frac{n\pi}{a}\right)^2 + \delta^2\right] \pm |V_G|\left(1 + \left(\frac{\hbar^2 n\pi\delta}{ma|V_G|}\right)^2\right)^{\frac{1}{2}}$$

TAYLOR $\to$
$$= \frac{\hbar^2}{2m}\left(\frac{n\pi}{a}\right)^2 \pm |V_G| + \frac{\hbar\delta^2}{2m}\left[1 \pm \frac{\hbar^2}{m}\left(\frac{n\pi}{a}\right)^2 \times \frac{1}{|V_G|}\right]$$

THUS DISPERSION IS QUADRATIC NEAR BZ BOUNDARY, WITH ONE MODE POINTING UP AND ONE DOWN



ONE LAST NOTE: IF WE HAVE PARABOLIC BANDS

$$E_+(G+\delta) = \text{Const}_+ + \frac{\hbar^2\delta^2}{2m_+^*}$$

$$E_-(G+\delta) = \text{Const}_- - \frac{\hbar^2\delta^2}{2m_-^*}$$

WE CAN THINK OF THESE AS ACTING LIKE FREE ELECTRONS, BUT WITH A NEW "EFFECTIVE" MASS $m_\pm^*$

$$\boxed{m_\pm^* = \frac{m}{\left| 1 \pm \frac{\hbar^2 (\frac{n\pi}{a})^2}{m|V_G|} \right|}}$$

THIS IS SOMETHING WE SAW BEFORE WHEN LOOKING AT REAL HEAT CAPACITY DATA $\longrightarrow$ ELECTRONS ACTING TOGETHER ACT AS THOUGH THEY HAVE A DIFFERENT MASS THAN FREE ELECTRONS

ACTING TOGETHER ≠ INTERACTING

QUICK CHECK ON VALIDITY OF NEARLY FREE ELECTRONS. TREMENDOUSLY SUCCESSFUL THEORY WHICH WE CAN UNDERSTAND, BUT BUILT ON THE ASSUMPTION $V(\vec{r}) << K$

PUT IN REAL NUMBERS.

WE KNOW FROM SOMMERFELD

$$K = k_B T_F = \left(8.617 \times 10^{-5} \frac{eV}{K}\right)\left(10^4 K\right)$$

$1eV = 1.6 \times 10^{-19} J$

$$\sim 1 eV$$

HUGE ENERGIES, BUT NEED ESTIMATE FOR $V(\vec{r})$. WE KNOW INTERACTIONS ARE FROM COULOMB POTENTIALS (PLUS SCREENING, YADA, YADA)

$$V(r) \sim \frac{1}{4\pi\varepsilon_0} \frac{e^2}{\cancel{r^2}} \qquad r \sim 10^{-10} m$$

$$= \frac{\left(8.99 \times 10^9 \frac{Nm^2}{C^2}\right)\left(1.6 \times 10^{-19} C\right)^2}{\left(10^{-10} m\right)\left(1.6 \times 10^{-19} \frac{J}{eV}\right)}$$

$$\sim \frac{10^{10}}{10^{-10}} \cdot 1.6 \times 10^{-19} \sim 10 eV$$

UH-OH . . . .

NEXT LECTURE - TIGHT BINDING MODEL