CONSIDER AN ELECTRON PLASMA. CHARGE NEUTRALITY IS PROVIDED BY THE POSITIVELY CHARGED ION CORES (NOTE: JELLIUM MODEL = CONSTANT POSITIVE BACKGROUND)

THE HAMILTONIAN IS:

$$H = \underbrace{\sum \frac{p_i^2}{2m_e}}_{\text{KE}} + \underbrace{\frac{e^2}{\epsilon_B} \sum_{i>j} \frac{1}{|\vec{r}_i - \vec{r}_j|}}_{\text{COULOMB } e\text{-}e \text{ INTERACTION}} + \underbrace{\sum_i U(\vec{r}_i)}_{\text{INT. W/ ION CORES}}$$

USE LENGTH SCALE DEFINED BY

$$a = \frac{1}{\left(\frac{4}{3}\pi\rho\right)^{1/3}}$$

ρ = DENSITY (3 DIMENSIONS)

ENERGY SCALE DEFINED BY

$$E_{Ryd} = \frac{\hbar^2}{2m_e a_0^2}$$

$$a_0 = \frac{\hbar^2 \epsilon_B}{m_e e^2} \approx 0.5\,\text{Å}$$ VACUUM

Bohr radius

THEN,

$$\frac{H}{E_{RYD}} = \frac{1}{r_s^2}\sum_i |\vec{\nabla}_{\vec{x}_i}|^2 + \frac{2}{r_s}\sum_{i>j}\frac{1}{|\vec{x}_i - \vec{x}_j|} + \tilde{U}$$

$$\boxed{r_s = a/a_0}$$

IF $r_s \ll 1$

$\Rightarrow$ KE DOMINATES

REGIME WHERE RANDOM PHASE APPROXIMATI[ON] APPLIES

STANDARD METALS
RPA WORKS WELL

$$\begin{cases} \rho : 10^{22} - 10^{23}\ cm^{-3} \\ 2 \le r_s \le 6 \end{cases}$$

DOPED SEMICONDUCTORS ; $r_s \lesssim 1$

$$\begin{cases} a_0\ (GaAs) \sim 10^2\ \mathring{A} \\ \rho \sim 10^{18}\ cm^{-3},\quad r_s \sim 0.6 \end{cases}$$

IF POTENTIAL ENERGY CAN BE IGNORED, THE SOLUTIONS TO SCHRÖDINGER EQ. ARE SLATER DETERMINANTS:

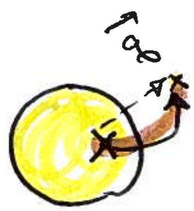
$$\Psi = \begin{vmatrix} \phi_1(\vec r_1,\hat\sigma_1) & \cdots & \phi_1(\vec r_N,\hat\sigma_N) \\ \vdots & & \vdots \\ \phi_N(\vec r_1,\hat\sigma_1) & \cdots & \phi_N(\vec r_N,\hat\sigma_N) \end{vmatrix}$$

(NOTE: Ψ CHANGES SIGN UNDER $\vec r_k \hat\sigma_k \leftrightarrow \vec r_p \hat\sigma_p$

GROUND STATE

$$\underbrace{2}_{\text{SPIN}} \times \left(\tfrac{4}{3}\pi k_F^3\right) = (2\pi)^3 \rho$$

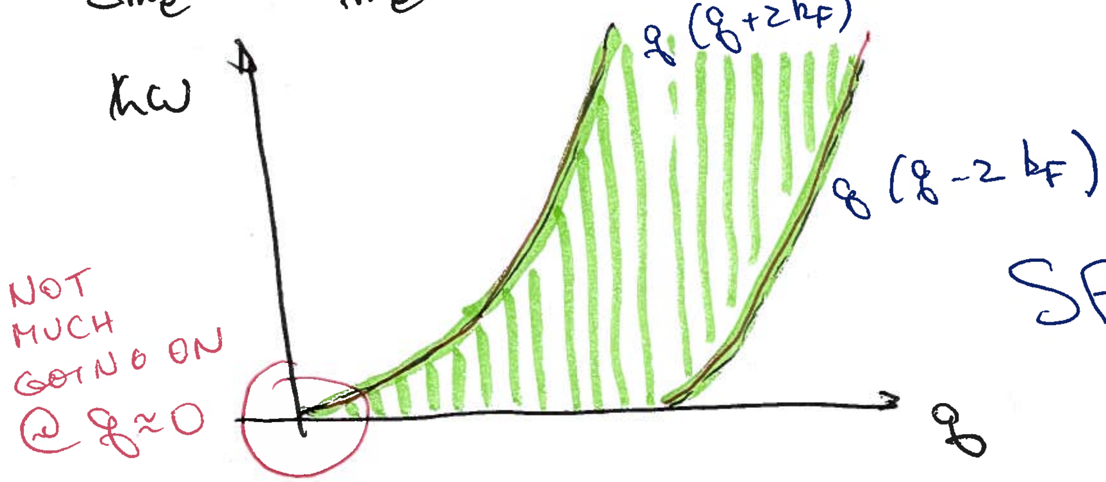
WHAT ARE THE EXCITATIONS ?



SINGLE-PARTICLE EXCITATIONS INVOLVE REMOVING 1 e @ $\vec k$ ($k < k_F$) & PLACING THE ELECTRON @ $\vec k'$ SO THAT $k' > k_F$

$$\hbar\omega = \frac{\hbar^2}{2m_e}(\vec q+\vec k)^2 - \frac{\hbar^2}{2m_e}k^2$$

$$= \frac{\hbar^2}{2m_e}q^2 + \frac{\hbar^2}{m_e}\vec q\cdot\vec k$$



SPE

TO DEAL WITH COULOMB INTERACTION, WE CALCULATE FIRST THE LONGITUDINAL PERMITTIVITY (DIELECTRIC CONSTANT)

THE HAMILTONIAN IS:

ELECTRON DENSITY OPERATOR

$$\hat{H} = \hat{H}_0 + \int \rho(\vec{r})\, \underbrace{\varphi_{ext}(\vec{r})}\, d^3r$$

ELECTROSTATIC POTENTIAL DUE TO EXTERNAL TEST CHARGE DISTRIBUTIO

$$\nabla^2 \varphi_{ext} = -\frac{4\pi}{\epsilon_B}\rho_{ext}$$

$$= -\frac{4\pi e}{\epsilon_B}\left[\Theta_q\, e^{-i(\omega t + \vec{q}\cdot\vec{r})} + c.c.\right]$$

$$\Rightarrow \varphi_{ext} = \frac{4\pi e}{\epsilon_B q^2}\left[\Theta_q\, e^{-i(\omega t + \vec{q}\cdot\vec{r})} + c.c.\right]$$

$$\rho(\vec{r}) = e \sum_i \delta(\vec{r} - \vec{r}_i)$$

$$\Rightarrow H_{INTERACTION} = \frac{4\pi e^2}{\epsilon_B q^2}\sum_i \left[\Theta_q\, e^{-i(\omega t + \vec{q}\cdot\vec{r}_i)} + c.c.\right]$$

INTRODUCE

$$\hat{\rho}_{\vec{q}} = \sum_i e^{i\vec{q}\cdot\vec{r}_i}$$

$$\Rightarrow \quad H_{\text{INTERACTION}} = \frac{4\pi e^2}{\epsilon_B q^2}\left[\underbrace{\Theta_q}_{\text{CONSTANT}}\hat{\rho}_{-q}\, e^{-i\omega t} + c.c.\right]$$

THE EXTERNAL FIELD INDUCES A NON-VANISHING VALUE OF

$$\langle \rho_{\vec{q}} \rangle$$

(MUCH IN THE SAME WAY THE COUPLING $\vec{A}_0 \cdot \hat{\vec{P}}$ LED TO AN INDUCED DIPOLE)

CAN BE CALCULATED USING PERTURBATION THEORY. WE'LL DO THIS IN A MINUTE. ASSUME WE HAVE ALREADY DONE IT.

THE INDUCED CHARGE DENSITY IS

$$\left[e\langle \rho_{\vec{q}} \rangle e^{+i(\vec{q}\cdot\vec{r}+\omega t)} + c.c.\right]$$

$\Downarrow$ QUASI-STATIC FIELDS

THE INDUCED ELECTROSTATIC POTENTIAL IS

$$\varphi_{\text{INDUCED}} = \frac{4\pi e}{\epsilon_B q^2}\left[\langle \rho_{\vec{q}} \rangle e^{i(\vec{q}\cdot\vec{r}+\omega t)} + c.c.\right]$$

USE MAXWELL'S EQS.

$$\begin{cases} \vec{\nabla}\cdot\vec{D} = 4\pi\,(\text{external charges}) \\ \vec{\nabla}\cdot\vec{E} = 4\pi\,(\text{external charges} + \text{induced charges}) \end{cases}$$

$$\Rightarrow \begin{cases} \vec{\nabla}\cdot\vec{D} = q^2 \varphi_{ext} \\ \vec{\nabla}\cdot\vec{E} = q^2(\varphi_{ext} + \varphi_{ind}) \end{cases}$$

SOLUTIONS

$$\begin{cases} \vec{D} = \left[D_{\vec{q}}\, e^{i(\vec{q}\cdot\vec{r}+\omega t)} + c.c. \right] \\ \vec{E} = \left[E_{\vec{q}}\, e^{i(\vec{q}\cdot\vec{r}+\omega t)} + c.c. \right] \end{cases}$$

$$\Downarrow$$

$$\begin{cases} i\,\vec{q}\cdot\vec{D}_q + c.c. = q^2 \varphi_{ext} \\ i\,\vec{q}\cdot\vec{E}_{\vec{q}} + c.c. = q^2 \varphi_{total} \end{cases}$$

DEFINE $\quad \epsilon_L(\omega,\vec{q}) = D_{\vec{q}} / E_{\vec{q}}$

$$\Rightarrow \frac{1}{\epsilon_L(\omega,\vec{q})} = 1 + \frac{\varphi_{IND}}{\varphi_{ext}} = 1 + \frac{\langle \rho_{\vec{q}} \rangle}{\Theta_{\vec{q}}\, e^{+i\omega t}}$$

CALCULATE $\langle \rho_{\vec{q}} \rangle$:

$$\Psi = \Psi_0 - \sum_n \frac{4\pi e^2}{\epsilon_B \hbar q^2} \left\{ \theta_{\vec{q}} \frac{\langle n | \rho_{-\vec{q}} | 0 \rangle e^{-i\omega t}}{-\omega + \omega_{n0} - i\delta} \right.$$

FIRST-ORDER PERTURBATION ON WAVEFUNCTION

CAUSALITY

$$\left. + \theta^*_{\vec{q}} \frac{\langle n | \rho_{\vec{q}} | 0 \rangle e^{i\omega t}}{\omega + \omega_{n0} + i\delta} \right\} \Psi_n$$

$$\Rightarrow \langle \Psi | \rho_{\vec{q}} | \Psi \rangle \approx -\frac{4\pi e^2}{q^2} \theta_{\vec{q}} e^{+i\omega t}$$

$$\times \sum_n \frac{|\langle n | \rho_{\vec{q}} | 0 \rangle|^2}{\hbar^2} \left[\frac{1}{\omega + \omega_{n0}} + \frac{1}{-\omega + \omega_{n0}} \right]$$

$$\Downarrow$$

$$\frac{1}{\epsilon(\omega, \vec{q})} = 1 - 4\pi \frac{e^2}{\epsilon_B \hbar q^2} \sum_n |\langle n | \rho_{\vec{q}} | 0 \rangle|^2 \left[\frac{1}{\omega + \omega_{n0} + i\delta} + \frac{1}{-\omega + \omega_{n0} - i\delta} \right]$$

$$\equiv 1 - 4\pi \chi(\omega, \vec{q})$$

USING THAT

$$\frac{1}{x \mp i\delta} = \fint \frac{1}{x} \mp i\pi\,\delta(x)$$

$$\mathrm{Im}\left[\frac{1}{\epsilon_L(\omega,\vec{q})}\right] = \frac{4\pi^2 e^2}{\epsilon_B q^2} \sum_n |\langle n|\rho_{\vec{q}}|0\rangle|^2$$

$$\times \left[\delta(\omega+\omega_{n0}) - \delta(-\omega+\omega_{n0})\right]$$

LONGITUDINAL PERMITTIVITY
NO APPROXIMATIONS WERE INVOLVED
EXACT
ZEROS OF ϵ GIVE EIGENVALUES $\hbar\omega_{n0}$

VERY GENERAL, NOT VERY USEFUL -
IF WE TAKE $|n\rangle \equiv$ SLATER DETERMINANT
NOTHING NEW WILL RESULT

RPA:

$$\frac{1}{\epsilon} = 1 + \frac{\varphi_{IND}}{\varphi_{ext}}$$

ALWAYS EXACT

USING SLATER DETERMINANTS:

$$\frac{\varphi_{IND}}{\varphi_{ext}} = -4\pi \chi_0$$

FREE ELECTRON SUSCEPTIBILITY

HARTREE or HARTREE-FOCK

NON-INTERACTING ELECTRONS:

$$\varphi_{IND} = -4\pi \chi_0 \varphi_{EXT}$$

RPA:

$$\varphi_{IND} = -4\pi \chi_0 \underbrace{(\varphi_{EXT} + \varphi_{IND})}_{\varphi_{TOTAL}} \; !$$

MEAN-FIELD APPROXIMATION

- EACH FOURIER COMPONENT CAN BE TREATED INDEPENDENTLY

$$\Rightarrow \varphi_{IND} = \frac{-4\pi \chi_0}{1+4\pi\chi_0} \varphi_{EXT}$$

SINCE $(1+4\pi\chi_0)^{-1} = 1 - 4\pi\chi_0 + (4\pi\chi_0)^2 - \ldots$

THIS EXPRESSION CANNOT BE DERIVED USING FINITE PERTURBATION THEORY

RPA:

$$\frac{1}{\epsilon_{RPA}} = 1 - \frac{4\pi\chi_0}{1+4\pi\chi_0}$$

$$\Rightarrow \boxed{\epsilon_{RPA} = 1 + 4\pi\chi_0}$$

IT CAN BE CALCULATED EXACTLY

$\Rightarrow$ LINDHARD EXPRESSION

BEHAVIOR OF ϵ_{RPA} @ $q \approx 0$ & $\omega \gg \omega_{m0}$ (SINGLE-PARTICLE EXCITATIONS)

NOTE :

$\langle m | \rho_{\vec{q}} | 0 \rangle$ CONNECTS STATE @ $\vec{k}$ WITH STATE @ $\vec{k}+\vec{q}$

$\rho_{\vec{q}} \to \sum_i e^{i\vec{q}\cdot\vec{r}_i}$

$$\Rightarrow \epsilon_{RPA} = 1 - \frac{8\pi e^2}{\epsilon_B \hbar q^2} \frac{1}{V_{CRYSTAL}} \sum_{k<k_F} \frac{\omega_{m0}}{\omega^2 - \omega_{m0}^2}$$

SINGLE-PARTICLE EXCITATIONS

EXPAND:

$$\epsilon_{RPA} \approx 1 - \frac{8\pi e^2}{\epsilon_B \hbar q^2} \frac{1}{\omega^2} \left[\frac{1}{V_c} \sum_m \omega_{m0} \right] - \frac{8\pi e^2}{\hbar q^2} \frac{1}{\omega^4} \times$$

$$\left[\times \frac{1}{V_c} \sum_m \omega_{m0}^3 \right] + \dots$$

$$\frac{1}{V_c}\sum_{m0}\omega_{m0} = \frac{1}{\hbar}\frac{1}{V_c}\frac{\hbar^2}{2m_e}\times$$

$$\times\sum_{k<k_F}\left(\cancelto{0}{2\vec{k}\cdot\vec{q}} + q^2\right) \equiv$$

$$\equiv \frac{\hbar q^2}{2m_e}\frac{N}{V_c}$$

$$\frac{1}{V_c}\sum_{m0}\omega_{m0}^3 = \frac{\hbar}{2m_e}\frac{1}{V_c}\sum_{k<k_F}\left(2\vec{k}\cdot\vec{q} + q^2\right)^3$$

$$\approx \frac{\hbar}{2m_e}\frac{1}{V_c}\sum_{k<k_F} 12(k\cdot q)^2 q^2 \propto q^4$$

THUS

$$\epsilon_{RPA} \approx 1 - \frac{4\pi e^2}{\epsilon_B\,\omega^2} N/V_c - \frac{8\pi e^2}{\epsilon_B\,\hbar\,\omega^4}\,C\,q^2 + \cdots$$

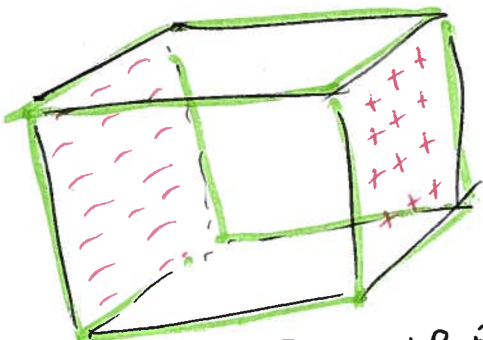
WHAT ARE THE ZEROS OF ϵ_{RPA}?

$$\omega \doteq \omega_p \left\{ 1 + \frac{3}{10} q^2 \frac{v_F^2}{\omega_p^2} + \cdots \right\}$$

$$\omega_p^2 = \frac{4\pi n e^2}{\epsilon_B m_e}$$

PLASMONS

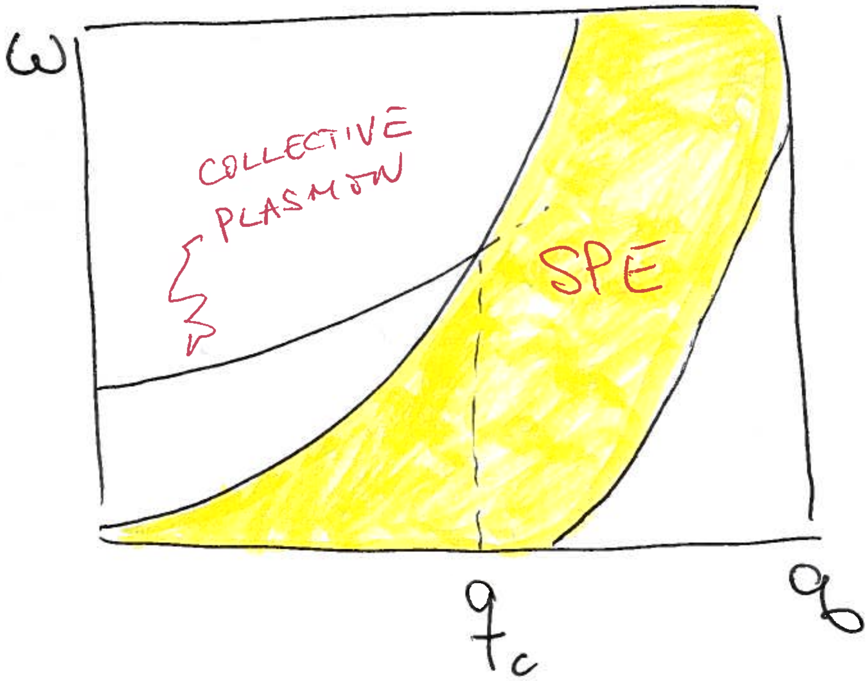
$\Rightarrow$ COLLECTIVE MODE OF ELECTRON SYSTEM



$E = 4\pi n e \delta$

SIMPLE PICTURE: $m\ddot{\delta} = -eE = -4\pi n \frac{e^2}{\epsilon_B} \delta$

$\Rightarrow \ddot{\delta} + \omega_p^2 \delta = 0$



LANDAU DAMPING

$q > q_c \approx k$

(SCREENING LENGTH^{-1}; SEE LATER)

BEHAVIOR @ $\omega = 0$

$$\epsilon_{RPA}(\omega=0, q) = 1 + \frac{8\pi m_e e^2}{\epsilon_B \hbar q^2} \times$$

$$\times \frac{1}{V_c} \sum_{\substack{k<k_F \\ |\vec{k}+\vec{q}|>k_F}} \frac{1}{(2\vec{k}\cdot\vec{q}+q^2)}$$

RESULT

$$\epsilon_{RPA}(q) = 1 + \frac{4\pi}{q^2} \frac{e^2 m k_F}{\epsilon_B \hbar^2 \pi^2} \left\{ \frac{1}{2} + \frac{1-x^2}{4x} \ln \frac{1+x}{1-x} \right\}$$

$$x = q/2k_F$$

FOR $x \ll 1$ $\left\{ \frac{1}{2} + \dots \right\} = 1$

$$\Rightarrow \underbrace{\epsilon_{RPA} \simeq 1 + \frac{k_0^2}{q^2}}_{\text{THOMAS-FERMI SCREENING}} \qquad k_0^2 = \frac{4\pi e^2 m_e k_F}{\hbar^2 \pi^2 \epsilon_B}$$

MEANING ?

IF $\varphi_{ext} = \frac{Q}{r} \Rightarrow \varphi_{ext}(q) = \frac{4\pi Q}{q^2}$

$$\Rightarrow \varphi_{TOTAL} = \frac{1}{\epsilon}\varphi_{ext} = \frac{4\pi Q}{q^2 + k_0^2}$$

$$\Rightarrow \varphi_{TOTAL}(r) = \frac{Q}{r} e^{-k_0 r}$$

YUKAWA POTENTIA[L]

$$k_0 \equiv \frac{2.95\,\text{Å}^{-1}}{(r_s/a_0)^{1/2}}$$

SCREENING IS VERY EFFECTIVE:

METALS: $k_0^{-1} \sim 0.5\,\text{Å}$

$n \sim 10^{17}\,\text{cm}^{-3}$ SEMICON: $k_0^{-1} \sim 5\,\text{Å}$

ANOTHER FEATURE OF LINDHARDT FUNCTION IS THAT

$$\varphi_{TOTAL}(r) \sim \frac{1}{r^3}\cos 2k_F r \quad \left(r \gg \frac{1}{k_0^{-1}}\right)$$

RUDERMAN-KITTEL or FRIEDEL OSCILLATIO[NS]

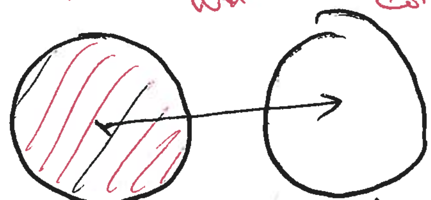
FINALLY $\partial G_{RPA}/\partial q \to \infty$ @ $q = 2k_F$

REAL EFFECT (KOHN EFFECT)

CONTRIBUTES TO E_{RPA}

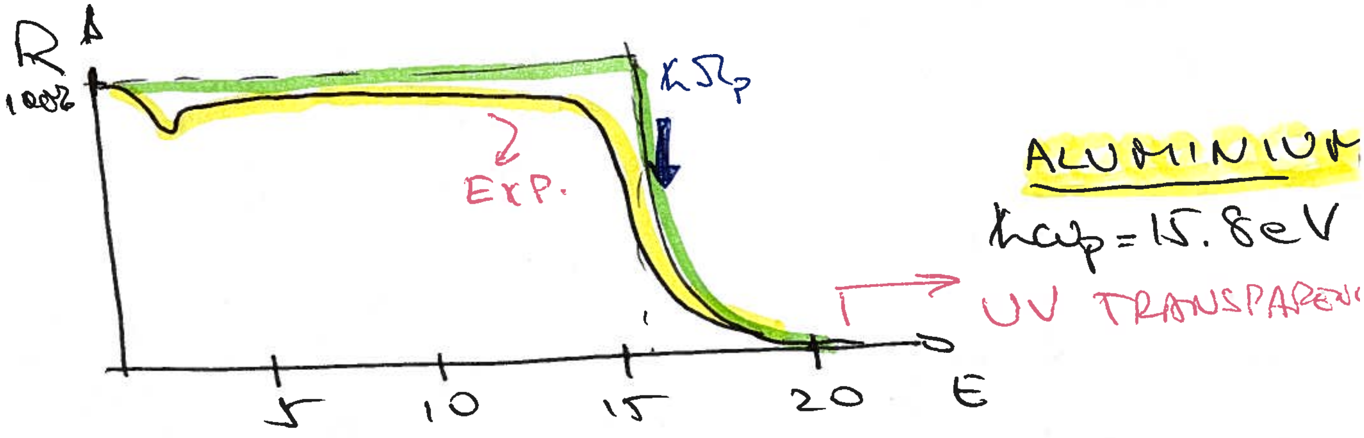
$q < 2k_F$

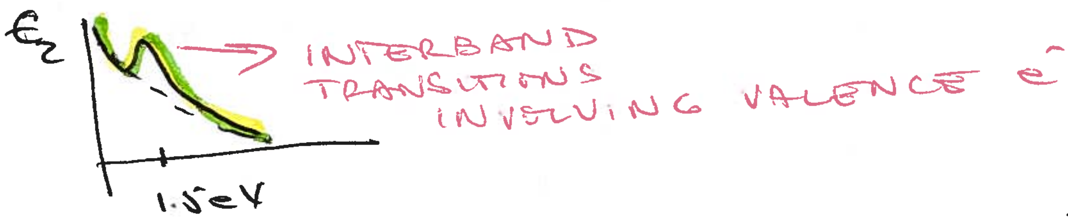
WHOLE SPHERE CONTRIBUTES



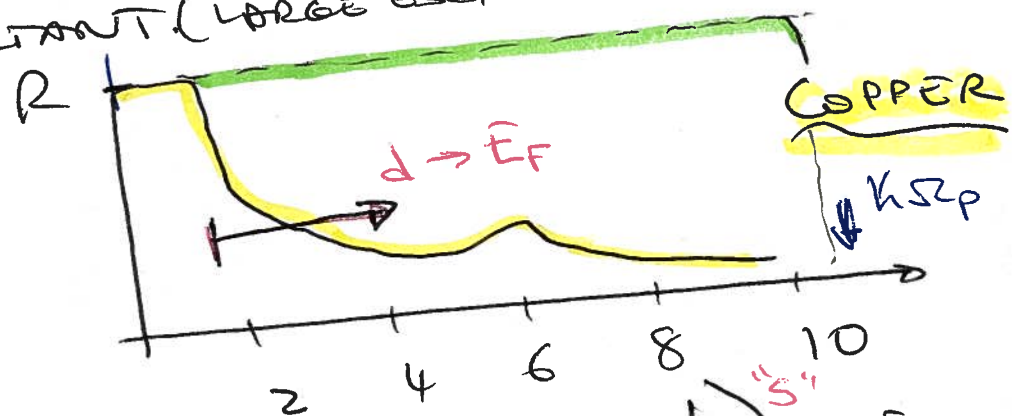
$q > 2k_F$

THE BEHAVIOR OF ACTUAL METALS DIFFERS FROM THAT PREDICTED BY DRUDE'S MODEL B'CAUSE OF INTERBAND TRANSITIONS

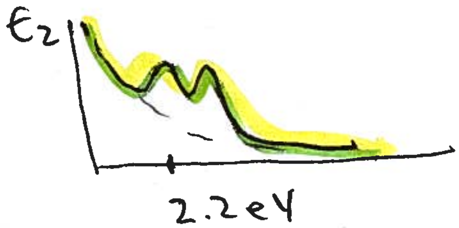


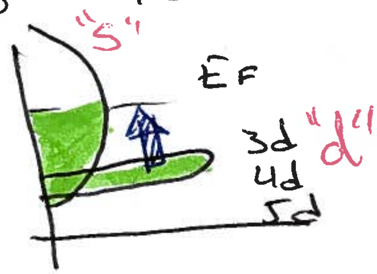


THINGS ARE SIGNIFICANTLY DIFFERENT FOR NOBLE METALS, FOR WHICH $d \to E_F$ TRANSITIONS ARE VERY IMPORTANT (LARGE OSCILLATOR STRENGTH)



NOBLE METAL	$d \to E_F$
Cu	~2.2eV
Au	~3eV
Ag	~4eV





SIMILAR EFFECTS CAN BE SEEN IN p-Ge, etc.