INTERBAND TRANSITIONS

WE BEGIN WITH THE EXPRESSION FOR $\varepsilon_2(\omega)$:

$$\varepsilon_2 = 4\pi \chi_2$$

ε_1 CAN BE FOUND USING KKR

(FOR ELECTRONS, $M_k \equiv m_e$, $Z \equiv 1$)

$$\varepsilon_2 = \frac{2\pi^2 e^2}{\hbar \omega^2 m^2} \frac{1}{V} \sum_m \left| \langle \psi_m | \sum_k P_k | \psi_{0s} \rangle \right|^2$$

$$\left[\delta(\omega - \omega_m) + \delta(\omega + \omega_m)\right]$$

WHAT IS ψ_m?

IT IS A SLATER ~~DETERMINANT~~ INVOLVING ALL STATES OCCUPIED BY ELECTRONS

BECAUSE $\sum_k \vec{P}_k \equiv -i\hbar \sum_k \vec{\nabla}_k$ IS A SINGLE ELECTRON OPERATOR

ψ_M CAN ONLY INVOLVE TRANSITION OF A SINGLE ELECTRON

$$\langle \psi_1(R_1) \ldots \psi_s(R_s') \ldots | \sum_k P_k | \psi_1(R_1) \ldots \psi_s(R_s) \psi_N(R_N) \rangle$$

ALL BUT ONE ARE THE SAME

THEREFORE, EXCEPT FOR NORMALIZATION FACTORS

$$\left| \langle \Psi_{fm} | \sum_k p_k | \Psi_{os} \rangle \right|^2 \propto$$

$$\propto \left| \hat{n} \cdot \langle \psi_j^{(s')} | -i\hbar \vec{\nabla} | \psi_i^{(s)} \rangle \right|^2$$

polarization of ELECTRIC FIELD

BLOCH FUNCTIONS

BAND INDEX

$$\int e^{-i\vec{k}_j \cdot \vec{r}} u_{k_j}^{s'*}(\vec{r}) \, \vec{\nabla} \left\{ e^{i\vec{k}_i \cdot \vec{r}} u_{k_i}^{s}(\vec{r}) \right\} d^3 r$$

REQUIRES THAT $\vec{k}_j \equiv \vec{k}_i$ (VERTICAL TRANSITIONS)

$\equiv$ DIPOLE APPROXIMATION

MATRIX ELEMENT

$$i k_i \cancel{\int u_{k_j}^{(s)*}(r) \, u_{k_i}^{s'} \, d^3 r} + \int u_{k_j}^{(s')*} \vec{\nabla} u_{k_i}(\vec{r}) \, d^3 r$$

$$0$$

THUS, WE GET

$$\varepsilon_2 = \frac{2\pi^2 e^2 \hbar^2}{m^2 \omega^2} \frac{1}{V} \times$$

$$\times \sum_{\substack{\vec{k} \\ s:\text{OCCUPIED} \\ s':\text{EMPTY}}} \left| m_0 \langle \psi_{\vec{k}}^{(s')} | \vec{\nabla} | \psi_{k}^{(s)} \rangle \right|^2 \left\{ \delta\left[\hbar\omega - E_{s'}(\vec{k}) + E_s(\vec{k})\right] + \delta\left[\hbar\omega + E_{s'}(\vec{k}) - E_s(\vec{k})\right] \right\}$$

EMISSION

$$\boxed{\sum_{\vec{k}} \equiv \frac{V}{8\pi^3} \iiint dk_x\, dk_y\, dk_z}$$

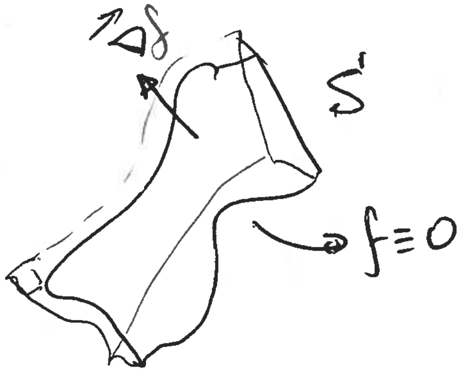
$$\varepsilon_2 = \frac{e^2 \hbar^2}{4\pi \omega^2 m^2} \int_{BZ} dk_x\, dk_y\, dk_z \; \left| \langle s' | \vec{\nabla} | s \rangle \right|^2 \delta\left[\hbar\omega - E_{s'}(\vec{k}) + E_s(\vec{k})\right]$$

$$\boxed{E_{s'}(k) - E_s(k) = \hbar\omega}$$

DEFINES A SURFACE

How do we calculate integrals of the form

$$\int d^3r\, U(\vec{r})\, \delta[f(\vec{r})] \quad ?$$



$$d^3r = dS'\, \underbrace{dl}_{\text{NORMAL TO } \vec{dS}}$$

$$\boxed{dl \equiv \frac{df}{|\vec{\nabla}_{\vec{r}} f|}}$$

$$\Rightarrow \int d^3k\, U(\vec{r})\, \delta(f)$$

$$\equiv \int_{S'} \frac{dS'_{\vec{k}}\, U(\vec{r} \in S')}{|\vec{\nabla} f|}$$

INTRODUCE DENSITY OF STATES FOR A SINGLE BAND

$$N(E) = \frac{1}{4\pi^3} \int \frac{dS'_{\vec{k}}}{|\vec{\nabla}_{\vec{k}} E(\vec{k})|}$$

INTRODUCE JOINT DENSITY OF STATES

$$N_{ss'}(E) = \frac{1}{4\pi^3} \int \frac{dS_k}{\left|\vec{\nabla}_k \left[E_{s'}(\vec{k}) - E_s(\vec{k})\right]\right|}$$

$$\Rightarrow \quad \varepsilon_2 = \frac{e^2\hbar^2}{4\pi\omega^2 m^2} \int_S \frac{\left|\langle s'|\vec{\nabla}|s\rangle_k\right|^2 \, dS_k}{\left|\vec{\nabla}_k \left[E_s - E_{s'} + \hbar\omega\right]\right|}$$

IF MATRIX ELEMENTS VARY WEAKLY WITH ENERGY, THEN

$$\boxed{\varepsilon_2 = \frac{e^2\hbar^2\pi^2}{\omega^2 m^2} N_{ss'}(E)} \times \left|\langle s'|\vec{\nabla}|s\rangle\right|^2$$

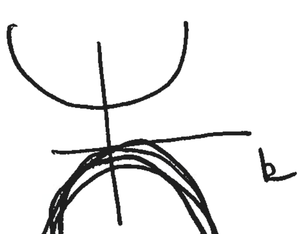
CRITICAL POINTS

INTEGRAL HAS SINGULARITIES AT POINTS FOR WHICH

$$\vec{\nabla}_k E_s = \vec{\nabla}_k E_{s'}$$

SIMPLEST CASE:

2 PARABOLIC BANDS @ $k = 0$



$$\begin{cases} E_{s'} = E_G + \alpha_{s'} k^2 \\ E_s = -\alpha_s k^2 \end{cases}$$

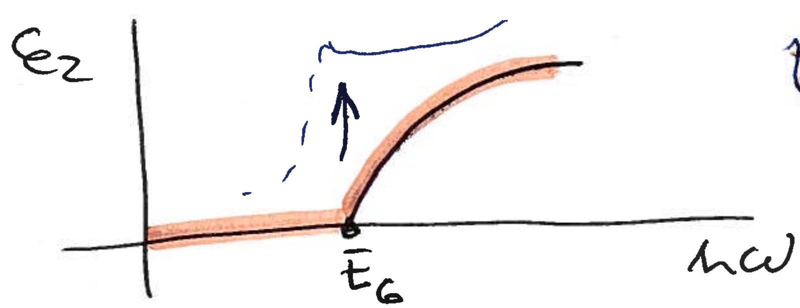
$$E_{s'} - E_s = \hbar\omega$$

$$E_G + (\alpha_s + \alpha')k^2 = \hbar\omega$$

$$|\vec{\nabla}_k| = 2(\alpha_s + \alpha')k = 2(\alpha_s + \alpha')^{1/2}\sqrt{\hbar\omega - E_G}$$

$$N_{ss'} \propto \int \frac{dk_x\, dk_y}{2(\alpha_s+\alpha')^{1/2}\sqrt{\hbar\omega - E_G}} \equiv \frac{\pi(\hbar\omega - E_G)}{2(\alpha_s+\alpha')^{3/2}(\sqrt{\hbar\omega - E_G})}$$

$$\propto \frac{\sqrt{\hbar\omega - E_G}}{(\alpha_s+\alpha')^{3/2}}$$



hard to see because of exciton effects

"M_0" CRITICAL POINT (3D)

ALSO WORKS IF

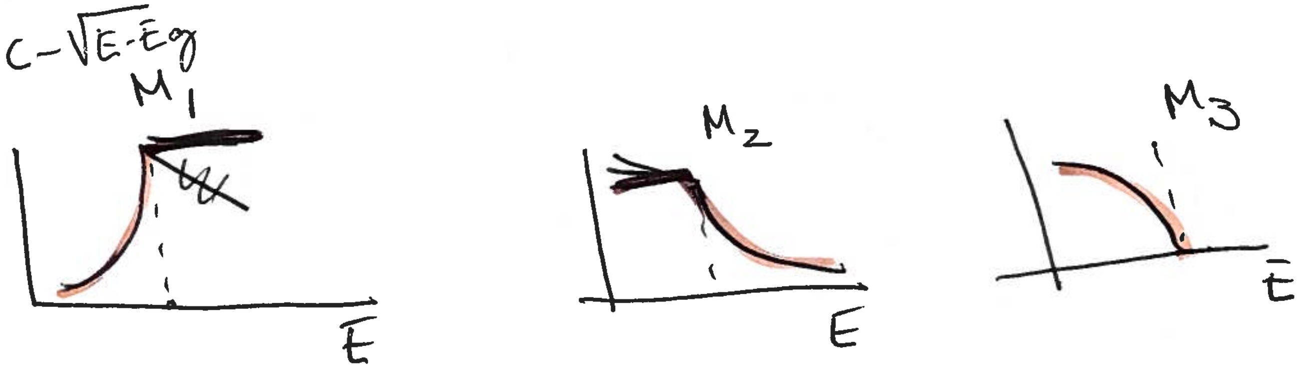
$$E = \alpha_1 k_x^2 + \alpha_2 k_x^2 + \alpha_3 k_z^2$$

$$E_{ss'} = E_{ss'}(0) + \alpha_1 k_x^2 + \alpha_2 k_y^2 + \alpha_3 k_z^2$$

IN 3D $\quad M_0, M_1, M_2, M_3$

$\alpha_i > 0 \qquad \alpha_1 < 0 \qquad \alpha_1, \alpha_2 < 0 \qquad \alpha_i < 0$

$\qquad\qquad\quad \alpha_2, \alpha_3 > 0 \qquad \alpha_3 < 0$



CALCULATE FOR $\underset{\sim}{M_1}$: (SADDLE POINT)

$$E_0 - \alpha k_x^2 + \beta(k_y^2 + k_z^2) = \hbar\omega$$

$(k_x - k_{x0}) \qquad (k_y - k_{y0}) \qquad (k_z - k_{z0})$

$$\vec{\nabla} E_{ss'} = (-2\alpha k_x, 2\beta k_y, 2\beta k_z)$$

$$N_{ss'} \propto \int_{S'} \frac{dS}{\sqrt{\alpha^2 k_x^2 + \beta^2(k_y^2 + k_z^2)}} \propto \int \frac{dS}{\sqrt{(\hbar\omega - E_0) + (\alpha^2 + \alpha\beta) k_x^2}}$$

$$\cancel{\propto \int \frac{dS}{\sqrt{\hbar\omega - E_0 + \beta(k_y^2 + k_z^2) k_x^2}}}$$

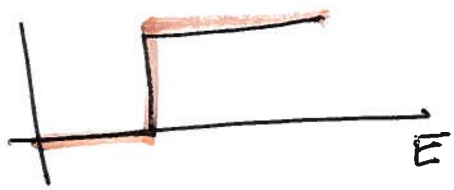
In 2D $\quad M_0, M_1, M_2$ (SAME MATH)

- $M_0 | M_2 \qquad \alpha(k_x^2 + k_y^2) = \hbar\omega - E_g$

"SURFACE" $\Rightarrow$ CURVE $\Rightarrow$ CIRCLE

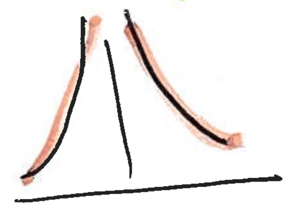
$\vec{\nabla} \propto (k_x, k_y)$

$$\Rightarrow \quad N_{SS'} \propto \int \frac{dS}{\sqrt{k_x^2 + k_y^2}} \propto \frac{2\pi\sqrt{\hbar\omega - E_g}}{\sqrt{\hbar\omega - E_g}} \equiv \text{const}$$



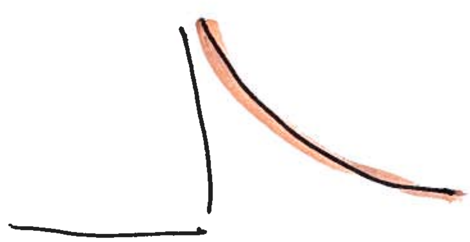
- $M_1 \qquad \alpha k_x^2 - \beta k_y^2 = \hbar\omega - E_g$

$\ln|\hbar\omega - E_g|$



E_g

FINALLY, IN 1D



$$\frac{1}{\sqrt{\hbar\omega - E_g}}$$

M_0, M_1