

EFFECTIVE-MASS THEORY

Lecture #7

8

ZIMAN, Ch. 6

+ JONES/MARCH
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LANDAU-LEVELS
FRANZ-KELDYSH EFF
~~WANNIERS~~

$$\hat{H} = H_0^{(0)} + \hat{V}(\vec{r}, t)$$

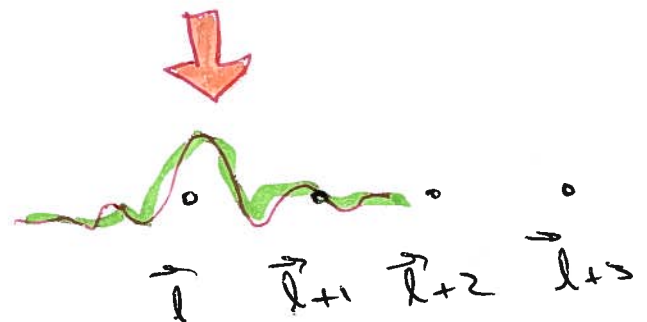
electron
in
periodic
lattice

external perturbation

$$\Psi = \sum_{\vec{l}} \overbrace{f_n(\vec{l}, t)}^{\text{envelope function}} \underbrace{a_n(\vec{r} - \vec{l})}_{\text{lattice site}}$$

n, \vec{l}
labels
a band

WANNIER
FUNCTION



$$a_n(\vec{r} - \vec{l}) = \frac{1}{N} \sum_{\vec{R}} e^{-i\vec{k} \cdot \vec{l}} \psi_{\vec{k}, n}(\vec{r})$$

$$\left[\epsilon_n(-i\vec{\nabla}) f_n - i\hbar \frac{\partial f_n}{\partial t} \right]_{\vec{l}} +$$

EXACT

$$+ \sum_{n' \neq n} V_{nn'}(\vec{l}, \vec{l}') f_{n'}(\vec{l}', t) = 0$$

TO GET EFF-MASS EQ.:

ASSUMPTIONS

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$$1. V_{mm'}(\vec{r}, \vec{r}') \approx V(\vec{r}) \quad \vec{r} = \vec{r}'$$

TRUE IF \hat{V} IS SLOWLY VARYING BECAUSE OF ORTHOGONALITY OF WANNIER FUNCTIONS

$$2. \epsilon(\vec{k}) \approx \frac{\hbar^2 k^2}{2m^*}$$

IGNORE HIGHER-ORDER TERMS

THEN

$$\left[-\frac{\hbar^2}{2m^*} \nabla^2 - i\hbar \frac{\partial}{\partial t} \right] f_m + \hat{V}(\vec{r}) f_m = 0$$

EFFECTIVE - MASS EQUATION

→
$$\psi_m \approx \sum_{\vec{l}, \vec{k}} \frac{f_m(\vec{l}, t)}{\sqrt{N}} e^{-i\vec{k} \cdot \vec{l}} \psi_{\vec{k}, m}(\vec{r})$$

$$\psi_n \approx \frac{1}{\sqrt{N}} \sum_{\vec{l}, \vec{k}} f_n(\vec{l}, t) e^{i\vec{k}(\vec{r}-\vec{l})} u_{\vec{k}, n}(\vec{r}) \quad (10)$$

SINCE \hat{V} IS SLOWLY VARYING THE FOURIER COMPONENTS OF f_n ARE NON-ZERO FOR $|\vec{k}| \sim \frac{1}{L} \downarrow$

$$\Rightarrow \psi_n \approx \underbrace{f_n(\vec{r}, t)}_{\text{ENVELOPE}} e^{i\vec{k}_0 \cdot \vec{r}} u_{\vec{k}=0, n}(\vec{r})$$

IF WE ARE INTERESTED IN VALUES OF $\vec{k} \neq 0$, SUCH THAT

$$E \approx E_0 + \frac{\hbar^2}{2m} (\vec{k} - \vec{k}_0)^2$$

$$\Rightarrow -\frac{\hbar^2}{2m} \left[e^{-i\vec{k}_0 \cdot \vec{r}} \frac{\partial}{\partial \vec{r}} e^{i\vec{k}_0 \cdot \vec{r}} \right]^2 f$$

$$-i\hbar \frac{\partial f}{\partial t} + \hat{V}(\vec{r}) f = 0$$

$$\Rightarrow -\frac{\hbar^2}{2m} \nabla^2 (e^{i\vec{k}_0 \cdot \vec{r}} f) + \hat{V} (e^{i\vec{k}_0 \cdot \vec{r}} f) = i\hbar \frac{\partial}{\partial t} (e^{i\vec{k}_0 \cdot \vec{r}} f)$$

SLOWLY VARYING

OPTICAL SELECTION RULES

(11)

$$\Psi_v = f_v(\vec{r}) u_v(\vec{r})$$



$f_{c,v}$: SLOWLY VARYING

$$\Psi_c = f_c(\vec{r}) u_c(\vec{r})$$

$$\langle \Psi_c | \vec{A}_0 \cdot \vec{p} | \Psi_v \rangle \approx \langle f_c | f_v \rangle \underbrace{\langle u_c | \vec{A}_0 \cdot \vec{p} | u_v \rangle}_{\text{ALREADY DISCUSSED}}$$

EXAMPLE # 1

LANDAU-LEVELS

FOR CONSTANT **MAGNETIC FIELD**, PARALLEL TO \hat{z}

TAKE $A_x = -B_0 y$ $A_y = A_z = 0$

(Alternatively, $\vec{A} = \frac{1}{2} \vec{B}_0 \times \vec{r}$)

ORIGINAL PROBLEM:

$$\hat{H} = \frac{1}{2m} \left[\left(\hat{p}_x + \frac{eB_0}{c} y \right)^2 + p_y^2 + p_z^2 \right] + \underbrace{U(\vec{r})}_{\text{PERIODIC POTENTIAL}}$$

BALE MASS



$$H_{\text{EFF}}^* = \frac{1}{2m^*} \left[\left(\hat{p}_x + \frac{eB_0}{c} y \right)^2 + p_y^2 + p_z^2 \right]$$

SOLUTIONS

(12)

$$\psi = e^{i/k [P_x^{(0)} x + P_z^{(0)} z]} \chi(y)$$

$$\frac{1}{2m^*} \left[\left(P_x^{(0)} + \frac{eB_0}{c} y \right)^2 - \hbar^2 \frac{d^2}{dy^2} + P_z^{(0)2} \right] \chi = E \chi$$

TAKE $y_0 = -\frac{P_x^{(0)} c}{eB_0}$

$$\omega_c = \frac{|e| B_0}{m^* c}$$



$$-\frac{d^2 \chi}{dy^2} + \frac{2m^*}{\hbar^2} \left[\left(E - \frac{P_z^{(0)2}}{2m^*} \right) - \frac{1}{2} m^* \omega_c^2 \right]$$

$$\left[(y - y_0)^2 \right] \chi = 0$$

HARMONIC OSCILLATOR
CENTERED @ $y = y_0$

$$\rightarrow E = \left(m + \frac{1}{2} \right) \hbar \omega_c + \frac{P_z^{(0)2}}{2m^*}$$

$$\psi_n(y) = C e^{-\frac{(y-y_0)^2}{2a_c^2}} H_n\left(\frac{y-y_0}{a_c}\right)$$

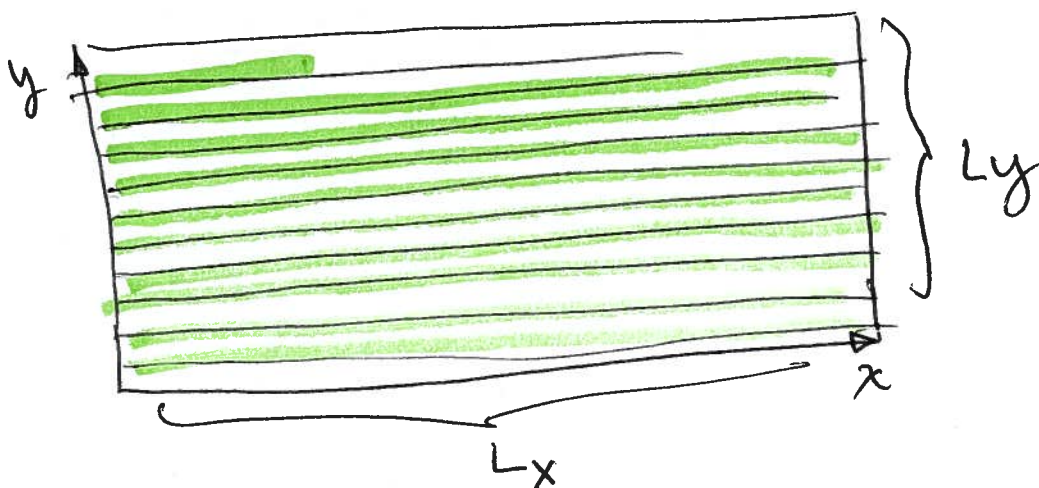
(13)

$$a_c = \sqrt{\frac{\hbar}{m\omega_c}}$$

HERMITE
POLYNOMIAL

CYCLOTRON LENGTH

FOR A FIXED n , SAY, $n=0$ ($\frac{1}{2}$ FIXED $P_z^{(0)}$)



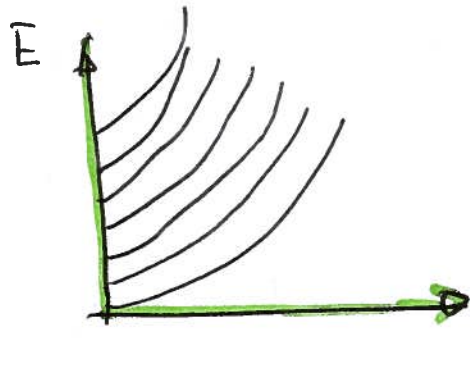
ENORMOUS DEGENERACY

$$\#_{\text{STATES}} = \frac{L_x L_y m^* \omega_c}{\hbar}$$

$$= \frac{L_x L_y (e\hbar) B_0}{\hbar c}$$

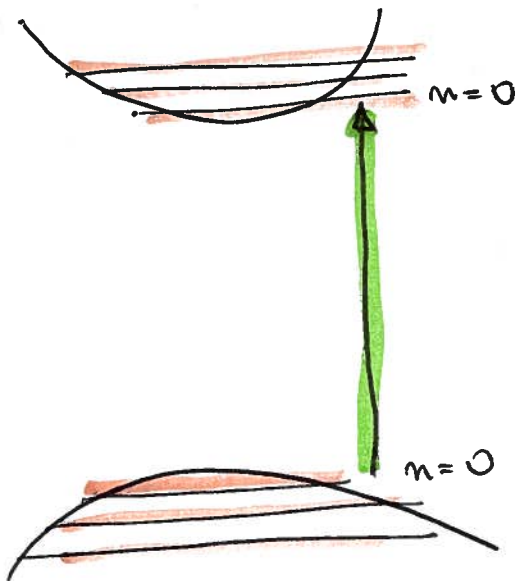
(INDEPENDENT
OF MASS)

$$\left\{ \frac{P_x^{(0)}}{\hbar} L_x \leq 1 \quad y_0 \leq L_y \right\}$$



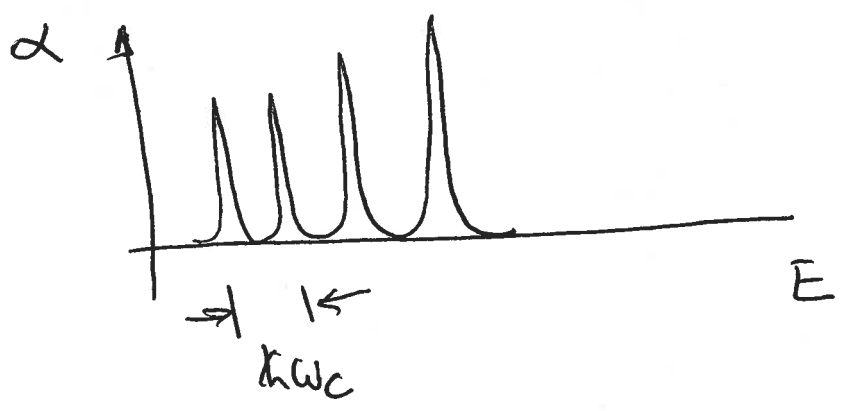
LIKE 1D PROBLEM !

OPTICAL SELECTION RULES :



ALL QUANTUM NUMBERS OF ENVELOPE FUNCTION MUST BE THE SAME

SAME γ_0 !



NOTE:

BECAUSE v.b IS NOT PARABOLIC, THINGS ARE MORE COMPLICATED FOR III-V COMPOUNDS

FRANZ-KELDYSH

(15)

ELECTRIC FIELD F_E

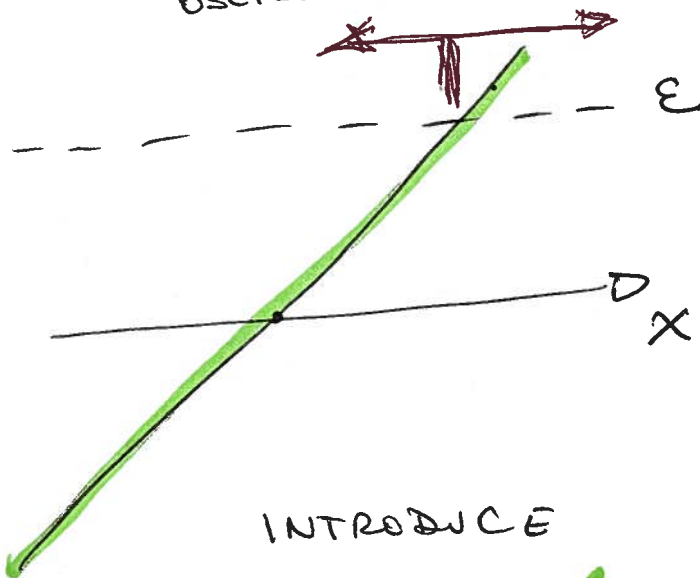
$$\alpha(\hbar\omega) \propto \begin{cases} \exp\left[-\frac{4\sqrt{2m^*}}{3|e|F_E\hbar} (E_g - \hbar\omega)^{3/2}\right] \\ \sin\left[\frac{2\sqrt{2m^*}}{3|e|F_E\hbar} (\hbar\omega - E_g)^{3/2} + \frac{\pi}{4}\right] \end{cases}$$

OSCILLATIONS
FOR $\hbar\omega > E_g$

EFFECTIVE HAMILTONIAN

$$-\frac{\hbar^2}{2m^*} \frac{d^2\psi}{dx^2} - e|F_E|x\psi = \epsilon\psi$$

OSCILLATES EXPONENTIAL DECAY



INTRODUCE

$$\xi = -\left(x + \frac{\epsilon}{|e|F_E}\right) / l$$

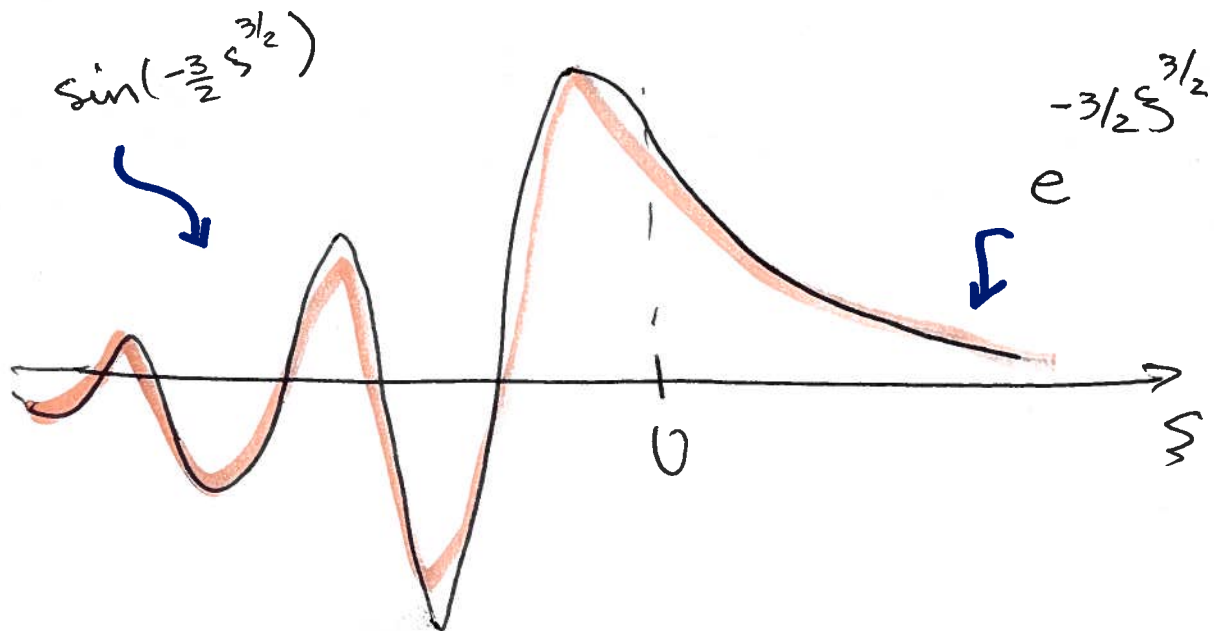
$$-\frac{\hbar^2}{2m^* l^2} \frac{d^2\psi}{d\xi^2} + |e|F_E l \xi \psi = 0$$

1F

$$l^3 = \frac{\hbar^2}{2m|e|Fe}$$

(16)

$$\Psi = \sum \Psi$$

AIRY FUNCTION


FOR LARGE $|\zeta|$, SOLUTIONS ARE OF THE FORM

$$\Psi \approx \zeta^{-1/4} e^{a|\zeta|^{3/2}} \quad a = \begin{cases} -3/2 \\ +i3/2 \end{cases}$$

HOW DOES THIS WORK?

IF $\frac{E}{eF_e} \gg$ length of sample

$\rightarrow |\psi(E)|^2$ PROBABILITY OF FINDING AND ELECTRON OF ENERGY E

~~ALTERNATIVELY~~ THUS, ORTHOGONAL IF $E_v \neq E_c$

$$\alpha \propto \sum_E |\langle u_c(\vec{p}, \vec{A}) | u_v \rangle|^2 \langle \psi_c | \psi_v \rangle_E \times \delta(\hbar\omega + E - E_c)$$

SINCE NOTHING CHANGES IN THE OTHER DIRECTIONS AND THE DENSITY OF STATES IS CONSTANT IN TWO DIMENSIONS, WE GET

$$\alpha \propto |\langle u_c(\vec{p}, \vec{A}) | u_v \rangle|^2 \cdot \underbrace{\psi^2 \left(\frac{E_c - \hbar\omega}{eEL} \right)}$$

$$e^{-4/3} \left[\frac{E_c - \hbar\omega}{eEL} \right]^{3/2}$$

A BETTER TREATMENT USES

$$E = -\frac{1}{c} \frac{\partial A}{\partial t} \quad \text{WITH} \quad \underline{A = -ctE_0}$$

\rightarrow L.V. KELDYSH, JETP 34, 788 (1958)

END OF DIRECT GAP ABSORPTION