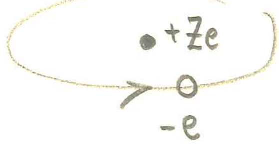
In This Lecture:

- ➢ **Spin-Orbit Interaction in Semiconductors**

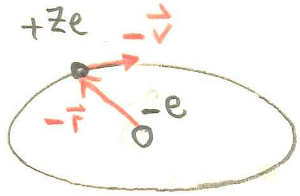
My apologies: This section is handwritten; too many equations ☹

Spin-orbit Interaction (Classical Approach)

Isolated Atom: Consider a single (or valence) e^- orbiting $+Ze$ ion



$\vec{r}, \vec{v}$



$\vec{r} \longrightarrow -\vec{r}$

$\vec{v} \longrightarrow -\vec{v}$

Lab frame

e- rest frame

Using Biot-Savart Law, at e^- site

$$\vec{B}_{eff} = \frac{\mu_0}{4\pi} Ze \frac{(-\vec{v}) \times (-\vec{r})}{r^3} = -\frac{\mu_0}{4\pi} \frac{Ze}{m_e} \frac{\hbar \vec{l}}{r^3}$$

$$m_e \vec{r} \times \vec{v} = \hbar \vec{l}$$

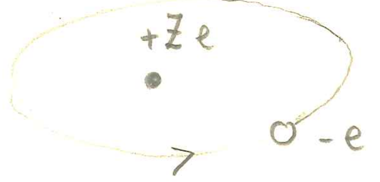
Using e^- spin magnetic moment

$$\vec{\mu}_s = -\overbrace{g_{e,s}}^{2} \mu_B \vec{s}, \quad \mu_B = \frac{e\hbar}{2m_e}$$

$$\therefore H_{so} = -\vec{\mu}_s \cdot \vec{B}_{eff} = -\frac{\mu_0}{4\pi} \frac{Ze^2}{2m_e^2} \frac{\hbar}{r^3} (\hbar \vec{l} \cdot \vec{s})$$

NB: This semiclassical treatment is off from Dirac eqn. (i.e., correct relativistic approach) by a factor of 2, the so-called Thomas factor

Let's now turn this into a form that we are familiar with. That is involving Electric field on the $\bar{e}$



$$\vec{E} = \frac{1}{4\pi\varepsilon_0} \frac{Ze}{r^3} \vec{r}$$

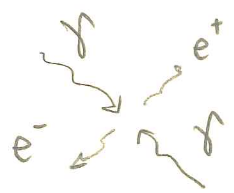
Also $\hbar \vec{l} = \vec{r} \times \vec{p}$

$$\therefore H_{so} = -\frac{\mu_0}{4\pi} \frac{Ze^2}{2m_e^2} \frac{\hbar}{r^3} (\hbar \vec{l} \cdot \vec{s}) \longrightarrow \frac{e\hbar}{2m_e^2 c^2} \vec{s} \cdot (\vec{p} \times \vec{E})$$

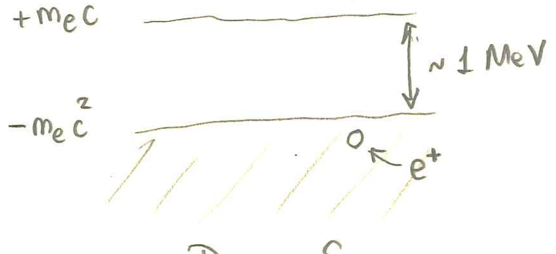
$\frac{1}{2}\vec{\sigma}$ $\quad -\frac{1}{e}\vec{\nabla} U$

$$\Rightarrow H_{so} = \frac{\lambda}{\hbar} \vec{\sigma} \cdot (\vec{p} \times \vec{\nabla} U), \quad \text{where } \lambda \equiv -\left(\frac{\hbar}{2m_e c}\right)^2$$

The denominator in H_{so} is $\propto 2m_e c^2 \simeq 1$ MeV which corresponds to particle-antiparticle energy gap



$2E_\gamma > 1$ MeV

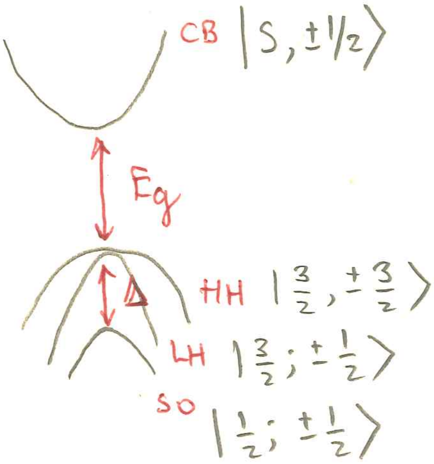


Dirac Sea

Semiconductors

1959 Roth et al showed within k.p and 2^{nd}-order perturbation theory that, the same form applies to semiconductors where λ value acquires a relation with E_g as opposed to particle-antiparticle gap.

$$H_{so} = \frac{\lambda}{\hbar}\, \vec{\sigma} \cdot \left(\vec{p} \times \vec{\nabla} U \right) , \quad \lambda = \frac{P^2}{3} \left[\frac{1}{E_g^2} - \frac{1}{(E_g + \Delta)^2} \right]$$



P : Kane's parameter $\langle S | p_x | X \rangle$

Time-reversal Symmetry

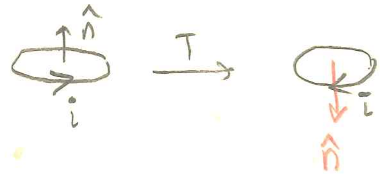
Zeeman Effect

$$\hat{H}_Z = -\hat{\vec{\mu}} \cdot \vec{B}$$

Under time-reversal operation $T: t \to -t$

$\vec{\mu} \longrightarrow -\vec{\mu}$ since $\vec{\mu} = \hat{n}\, i\, A$

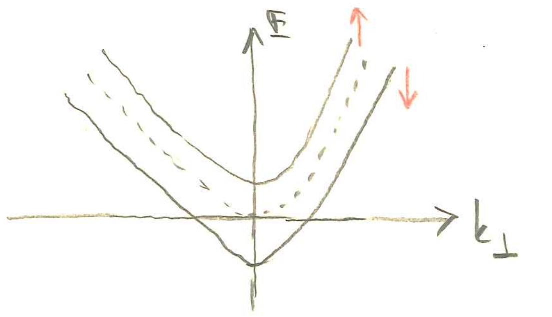
i: dq/dt



Note that even though $d\vec{B} \propto \dfrac{i\, \vec{dl} \times \vec{r}}{r^3}$ and under T: $\vec{B} \to -\vec{B}$

in Zeeman interaction $\vec{B}$ is an external field not a dynamical variable (i.e., operator), hence it is not affected by T

So, the presence of $\hat{H}_Z$ will break the time-reversal symm. and it causes a splitting bet. spin states $\uparrow, \downarrow$ along $\vec{B}$



Since $\hat{H}_{SOI}$ has a similar $\vec{S} \cdot \vec{B}_{eff} \to \vec{l} \cdot \vec{S}$ form:

→ Does SOI break time-reversal symmetry?

→ " " introduce a splitting bet. spin states?

$$T: \left.\begin{array}{l} t \to -t \\ \vec{\sigma} \to -\vec{\sigma} \\ \vec{l} \to -\vec{l} \end{array}\right\} \qquad \hat{H}_{SOI} \propto \vec{l}\cdot\vec{\sigma} \xrightarrow{T} \hat{H}_{SOI}$$

$\therefore$ SOI preserves time-reversal symmetry (unlike $\hat{H}_Z$)

* So, under T: $\vec{k} \to -\vec{k}$ and $\vec{\sigma} \to -\vec{\sigma}$

$$E_\uparrow(\vec{k}) = E_\downarrow(-\vec{k})$$

* If there is also space-inversion symmetry $\hat{H}(\vec{r}) = \hat{H}(-\vec{r})$

$$E_\uparrow(\vec{k}) = E_\uparrow(-\vec{k})$$

* Then, under time + space-inversion symmetry:

$$E_\uparrow(\vec{k}) = E_\downarrow(\vec{k}) \rightarrow \text{no spin splitting}$$

Therefore, to have spin selectivity, i.e., spin splitting we need

* time-inversion asymmetry $\Rightarrow$ ext. magnetic field

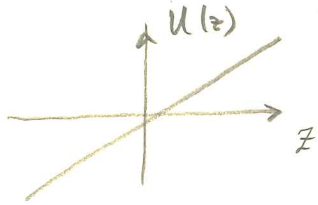
and/or

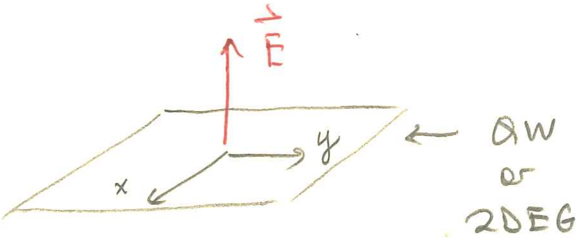
* space-inversion asymmetry
- $\rightarrow$ Bulk inversion asymm. – Dresselhaus
- $\rightarrow$ Structural " " – Rashba

Rashba Spin-orbit Interaction

In this case $-\vec{\nabla}U = e\vec{E}(\vec{r})$ is generated via an ext. potential (i.e. other than underlying xtal potential), such as a structural inversion asymmetry like DC field

$$U(\vec{r}) \to eEz$$





$$H_{RSO} = \frac{\lambda}{\hbar}\vec{\sigma}\cdot(\vec{p}\times \underbrace{\vec{\nabla}U}_{eE\hat{z}})$$

$$= \frac{eE\lambda}{\hbar}\left(p_y\sigma_x - p_x\sigma_y\right)$$

Here, we are considering SOI on the CB e^-'s via k.p coupling to VB

$$H_{RSO} = eE\lambda\left(k_y\sigma_x - k_x\sigma_y\right)$$

We can express this as:

$$H_{RSO} = \frac{\hbar}{2}\vec{\Omega}(\vec{k})\cdot\vec{\sigma} \; ; \quad \vec{\Omega}(\vec{k}) = 2\alpha_R\begin{pmatrix} k_y \\ -k_x \\ 0 \end{pmatrix}$$

with $\alpha_R = \dfrac{\hbar^2}{2m^*}\dfrac{\Delta}{E_g}\dfrac{2E_g+\Delta}{(E_g+\Delta)(3E_g+2\Delta)}eE$

can be tuned by ext. E-field

$$\alpha_R \to 0 \quad \text{for} \quad \begin{cases} E_g \to \infty & \text{(No VB coupling)} \\ \Delta \to 0 & \text{(No SOI in VB)} \end{cases}$$

Comparing vacuum (free atom) with se/c (say InAs)

$$E_{g,\,InAs} = 0.4\,eV \ll m_e c^2 = 0.5\,MeV$$

Also $m^*_{InAs} = 0.03\, m_e$

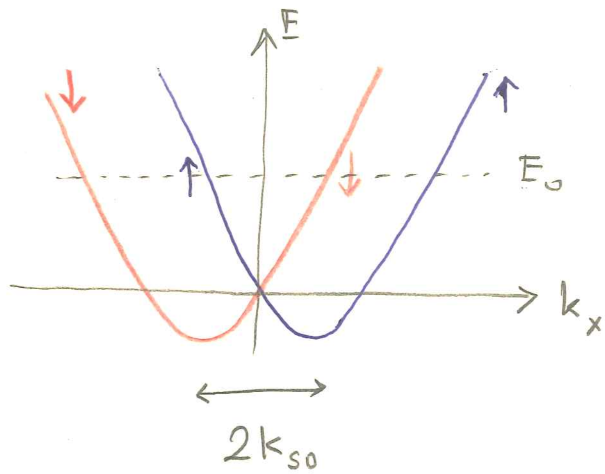
$\therefore$ $\alpha_{R,\,InAs}$ is about 10^7 times larger than in vacuum.

Dispersion diagram (CB):

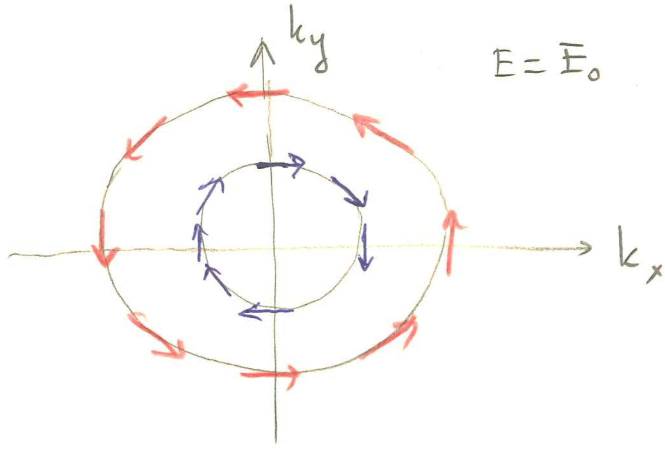
$$H = \frac{\hbar^2 k^2}{2m^*} + \alpha_R \begin{pmatrix} k_y \\ -k_x \\ 0 \end{pmatrix} \cdot \vec{\sigma}$$

minimum

$$k_{so} = \frac{m^* \alpha_R}{\hbar^2}$$



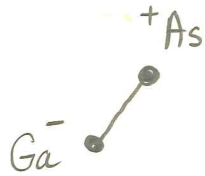
Spin-resolved isoenergy contours



Dresselhaus SOI

In this case the absence of inversion symmetry is due to (bulk) xtal structure, hence called bulk inversion asymmetry. As in Rashba SOI, we can express it for CB $\bar{e}$ in the form

$$H_{DSO} = \frac{\hbar}{2} \vec{\Omega}(\vec{k}) \cdot \vec{\sigma}$$



For bulk, as in ZB xtals like GaAs the anion-cation xtal field is responsible for BIA, which is not the case in diamond str, like Si. $\longrightarrow$ no BIA

In bulk xtals, the form of splitting is cubic in k (i.e., k^3)

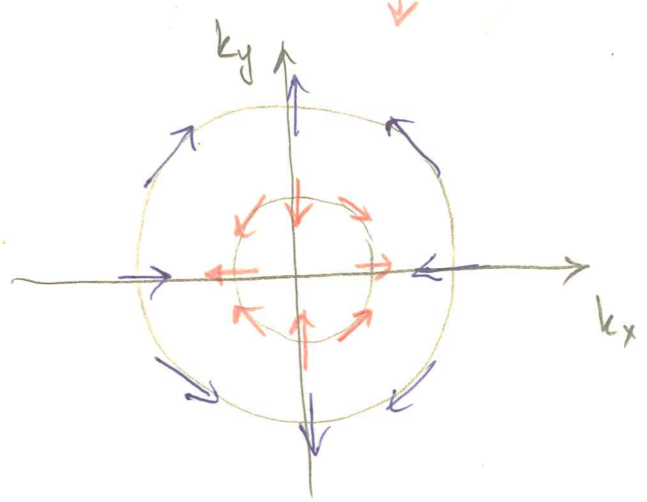
$$\vec{\Omega}(\vec{k}) = \gamma \begin{pmatrix} k_x (k_y^2 - k_z^2) \\ k_y (k_z^2 - k_x^2) \\ k_z (k_x^2 - k_y^2) \end{pmatrix}$$

In 2D str., say $\perp$ to $\hat{z}$: $k_z \rightarrow \langle \hat{k}_z \rangle = 0$, $k_z^2 \rightarrow \langle \hat{k}_z^2 \rangle$

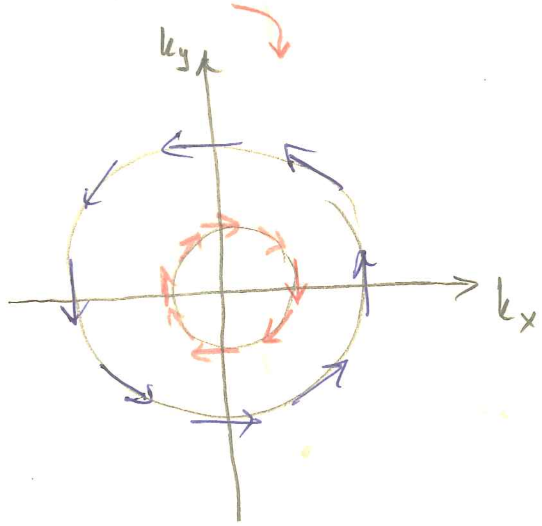
$$\vec{\Omega}(\vec{k}) = \gamma \langle k_z^2 \rangle \begin{pmatrix} -k_x \\ k_y \\ 0 \end{pmatrix} \sim \vec{k}$$

BIA can become particularly large in 2D case.

Dresselhaus (2D) vs Rashba SOI Isoenergy



$$\vec{\Omega}(\vec{k}) \sim \begin{pmatrix} -k_x \\ k_y \\ 0 \end{pmatrix}$$



$$\vec{\Omega}(\vec{k}) \sim \begin{pmatrix} k_y \\ -k_x \\ 0 \end{pmatrix}$$