2D Quantum Structures

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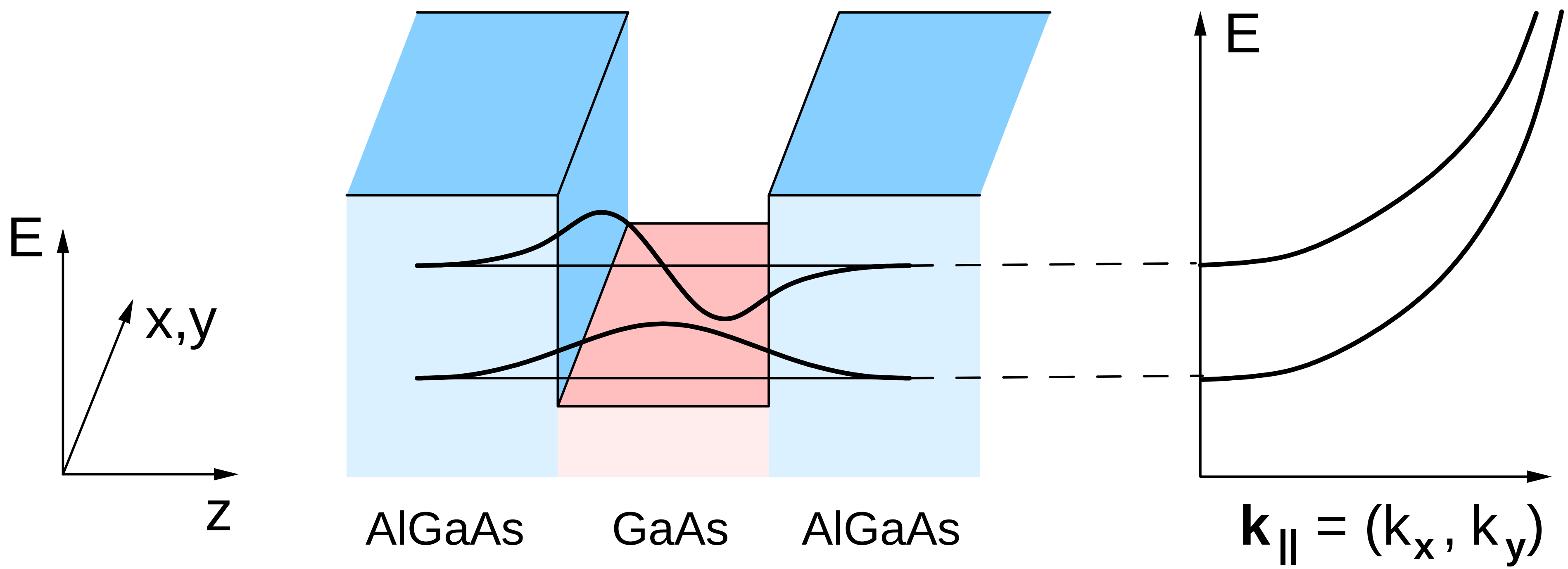


$$\hat{H} = \frac{p_x^2 + p_y^2}{2\,m^*} + \frac{p_z^2}{2\,m^*} + V(z)$$

$$E_n(\mathbf{k}_\parallel) = E_n + \frac{\hbar^2 k_\parallel^2}{2m^*}$$

$$\Psi_{n\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}_\parallel \cdot \mathbf{r}_\parallel}\, \xi_n(z)$$

Electrons in semiconductor quantum structures:

Envelope function approximation

Idea:

- Electrons in a semiconductor are free quasi particles

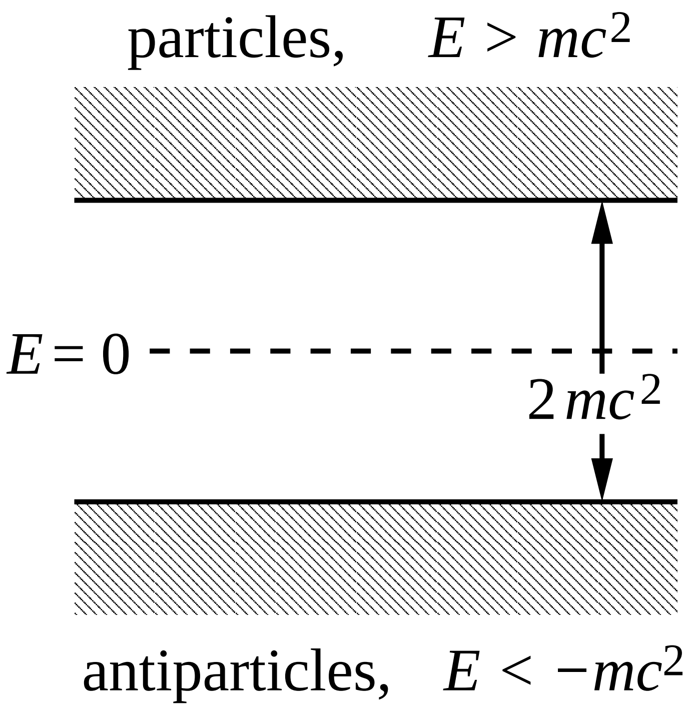
- Microscopic crystal structure
  $\longrightarrow$ effective quantities, e.g., $m \rightarrow m^*$
  $\Rightarrow$ dispersion $E(\mathbf{k}) = \dfrac{\hbar^2 k^2}{2m^*} + \mathcal{O}(k^3)$

- external potentials V: $\hbar\mathbf{k} \rightarrow -i\hbar\nabla$

  $\Rightarrow$ $\widehat{H} = E(-i\nabla) + V \approx -\dfrac{\hbar^2}{2m^*}\nabla^2 + V$
  $\Rightarrow$ envelope function $\Psi(\mathbf{r})$

- magnetic field: $h\mathbf{k} \rightarrow -ih\nabla + e\mathbf{A}$

Origin of Zeeman Splitting and Spin-Orbit Coupling (1)



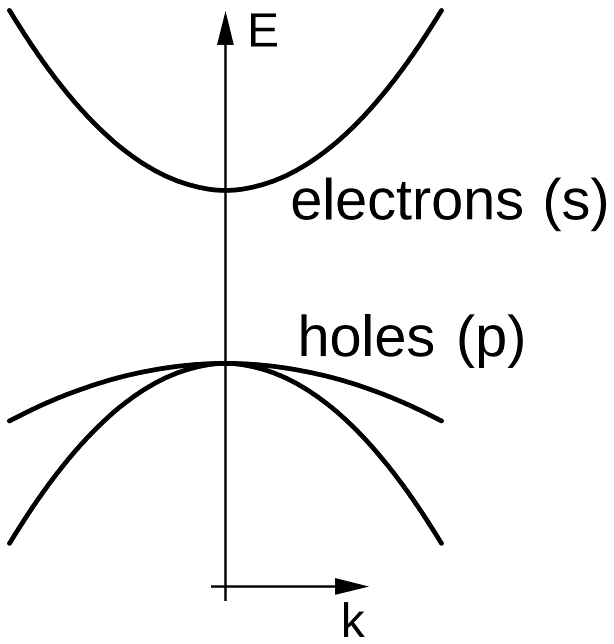
Relativistic Particle Physics

$\hookrightarrow$ decoupling particles and antiparticles

$\Rightarrow$ Pauli Equation

$H = \dfrac{p^2}{2m} + V$	kinetic and potential energy
$+ \dfrac{g}{2}\mu_\mathrm{B}\,\boldsymbol{\sigma}\cdot\mathrm{B}$	Zeeman term
$+ \dfrac{\hbar}{4m_0^2c^2}(\nabla V)\times\mathbf{p}\cdot\boldsymbol{\sigma}$	Pauli spin-orbit coupling

Origin of Zeeman Splitting and Spin-Orbit Coupling (2)



Semiconductors

$\hookrightarrow$ decoupling electrons and holes

$\Rightarrow$ effective Hamiltonian

$$H = \frac{p^2}{2m^*} + V$$ kinetic and potential energy

$$+ \frac{g^*}{2} \mu_{\mathrm{B}} \boldsymbol{\sigma} \cdot \mathbf{B}$$ Zeeman term

$$+ \alpha \, (\nabla V) \times \mathbf{p} \cdot \boldsymbol{\sigma}$$ Rashba spin-orbit coupling

Electrons (s-like)

strict one-to-one correspondence

particles $\Leftrightarrow$ electrons

Holes (p-like)

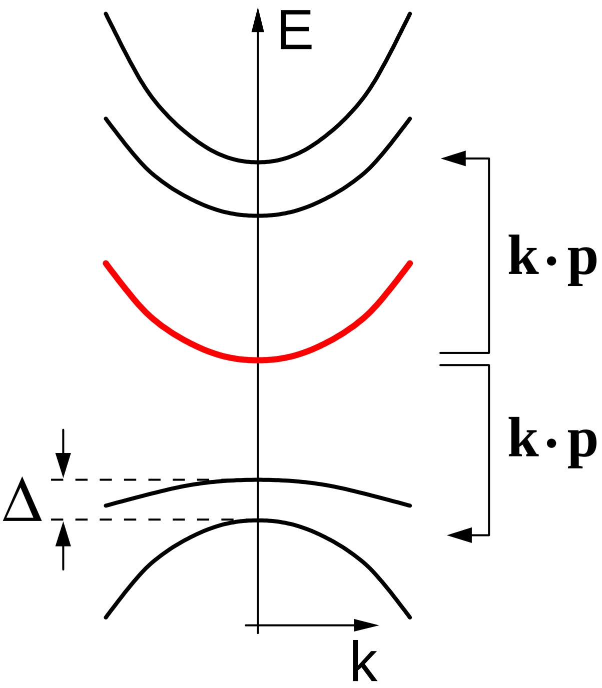
spin $s = 1/2$ | $j = 3/2$
orbital angular momentum $l = 1$ | & $j = 1/2$

Dispersion $E_\nu(\mathbf{k})$: $\mathbf{k}\cdot\mathbf{p}$ method

$$\left[\frac{\hat{p}^2}{2m_0} + \hat{V}_{\text{lattice}} + \hat{V}_{\text{SO}}\right] \psi_{\nu\mathbf{k}}(\mathbf{r}) = E_\nu(\mathbf{k})\, \psi_{\nu\mathbf{k}}(\mathbf{r})$$

with
$$\begin{aligned}\psi_{\nu\mathbf{k}}(\mathbf{r}) &= e^{i\mathbf{k}\mathbf{r}}\, u_{\nu\mathbf{k}}(\mathbf{r}) \\ &= e^{i\mathbf{k}\mathbf{r}} \sum_{n'} c_{\nu n'}(\mathbf{k})\, u_{n'\mathbf{0}}(\mathbf{r})\end{aligned}$$

$$\sum_{n'} \left[E_n(\mathbf{0})\, \delta_{nn'} + \frac{\hbar}{m_0}\, \mathbf{k}\cdot\mathbf{P}_{nn'} + \Delta_{nn'}\right] c_{\nu n'}(\mathbf{k}) = \\ = E_\nu(\mathbf{k})\, c_{\nu n}(\mathbf{k})$$



with

$$\mathbf{P}_{nn'} = \langle u_n |\, \hat{\mathbf{p}}\, | u_{n'} \rangle$$

$$\Delta_{nn'} = \langle u_n |\, \hat{V}_{\text{SO}}\, | u_{n'} \rangle$$

$\mathbf{k} = 0$: unperturbed band edge states

$\mathbf{k} \neq 0$: admixture of neighboring bands

$\mathbf{k} \ll 2\pi/a$ ($a =$ lattice constant)

$\Rightarrow$ perturbation theory for wave vector $\mathbf{k}$

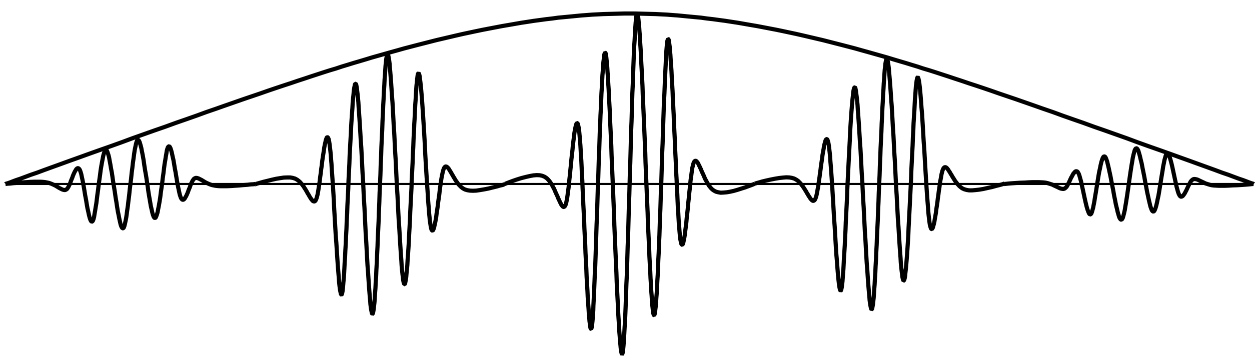
Envelope Function Approximation

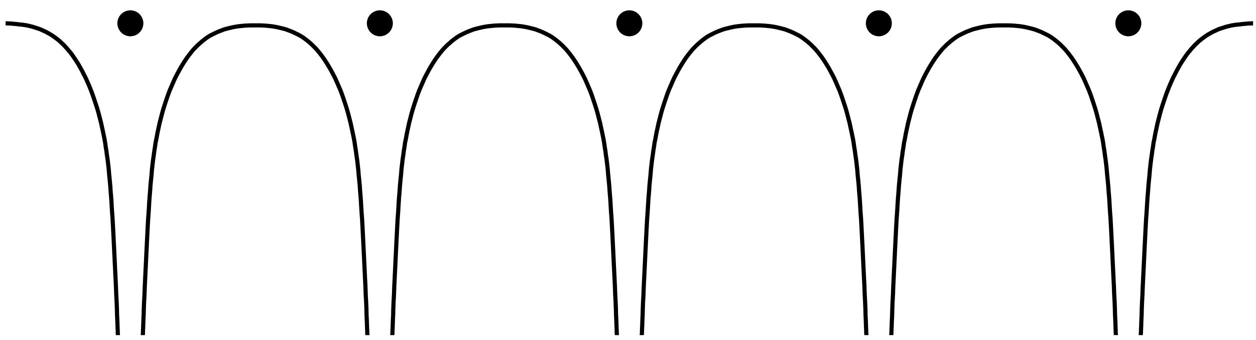
$$\left[\frac{\hat{p}^2}{2m_0} + \hat{V}_{\text{lattice}} + \hat{V}_{\text{SO}} + \hat{V}_{\text{ext}}\right] \Psi(\mathbf{r}) = E\,\Psi(\mathbf{r})$$

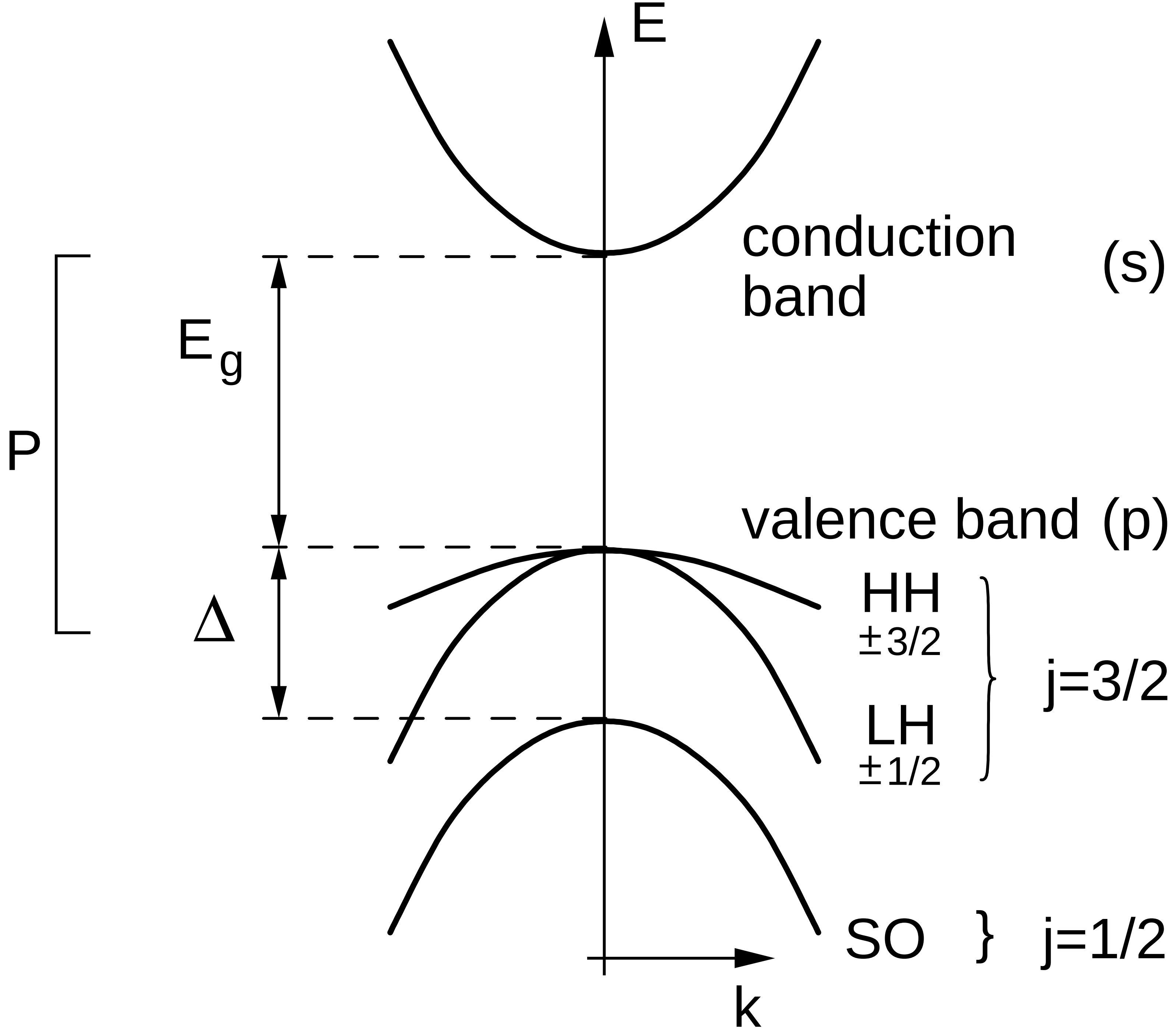
with $$\Psi(\mathbf{r}) = \sum_{n'} \phi_{n'}(\mathbf{r})\, u_{n'\mathbf{0}}(\mathbf{r})$$

$\hat{V}_{\text{ext}}$ slowly varying

$$\sum_{n'} \left[\left(E_n(\mathbf{0}) + \hat{V}_{\text{ext}}\right) \delta_{nn'} + \frac{\hbar}{m_0} (-i\nabla) \cdot \mathbf{P}_{nn'} + \Delta_{nn'} \right] \phi_{n'}(\mathbf{r}) = E\, \phi_n(\mathbf{r})$$






E
k
conduction band
(s)
valence band
(p)
E_g
P
Δ
HH
±3/2
LH
±1/2
j=3/2
SO
j=1/2

Orbital motion in an external potential V

- add V to the diagonal of $\mathbf{k}\cdot\mathbf{p}$ matrix
- $\hbar\mathbf{k} \;\rightarrow\; -i\hbar\nabla + e\mathbf{A}$

perturbative decoupling cb – vb
(similar to: Dirac equation → Pauli equation)

⇒ new terms in the conduction band:

(1) effective mass: $H_o = \frac{\hbar^2 k^2}{2m^*} + V$

with $$\frac{m_o}{m^*} \propto P^2 \left(\frac{2}{E_g} + \frac{1}{E_g + \Delta} \right)$$ (Kane, 1957)

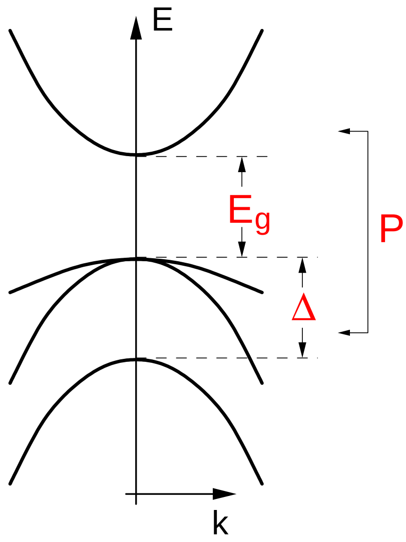
(2) $[k_x, k_y] = \frac{e}{i\hbar} B_z \quad \Rightarrow \quad H_{\mathrm{Zeeman}} = \frac{g^*}{2} \mu_{\mathrm{B}}\, \boldsymbol{\sigma} \cdot \mathbf{B}$

with $$g^* \propto P^2 \left(\frac{1}{E_g} - \frac{1}{E_g + \Delta} \right)$$ (Roth, 1959)

(3) $[\mathbf{k}, V] = -i\,\nabla V = -i\,e\boldsymbol{\mathcal{E}}$

⇒ $H_{\mathrm{Rashba}} = \alpha\, \mathbf{k} \times \boldsymbol{\mathcal{E}} \cdot \boldsymbol{\sigma}$

with $$\alpha \propto P^2 \left(\frac{1}{E_g^2} - \frac{1}{(E_g + \Delta)^2} \right)$$

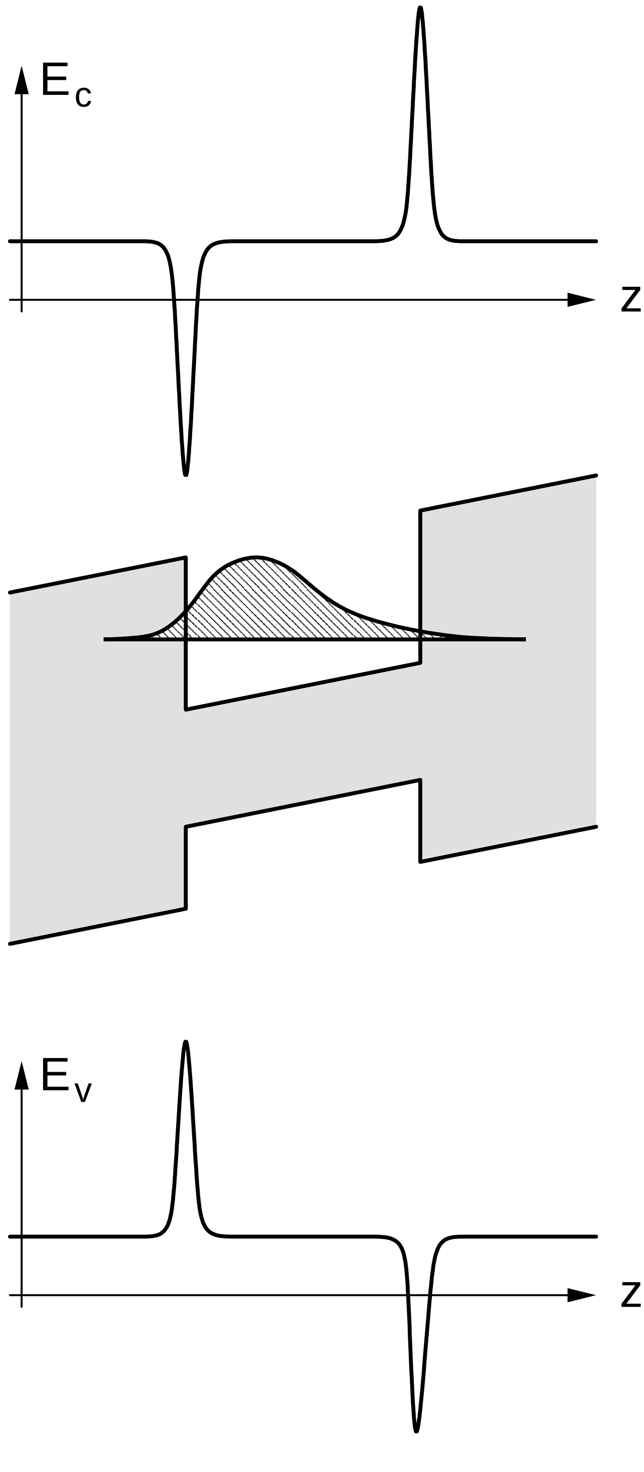


Rashba effect and Ehrenfest theorem

According to the Ehrenfest theorem: $\langle \mathcal{E} \rangle = 0$

"No force is acting on bound states"

Why is the Rashba effect not vanishing?



Due to the $\mathbf{k} \cdot \mathbf{p}$ coupling the electrons are sensing the electric field in the valence band

(Lassnig 1985)