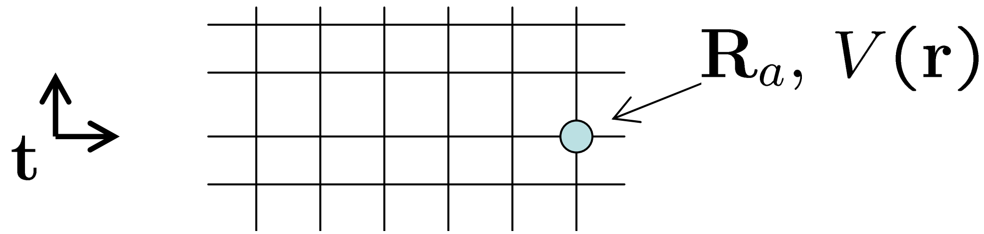
Spin-orbit coupling

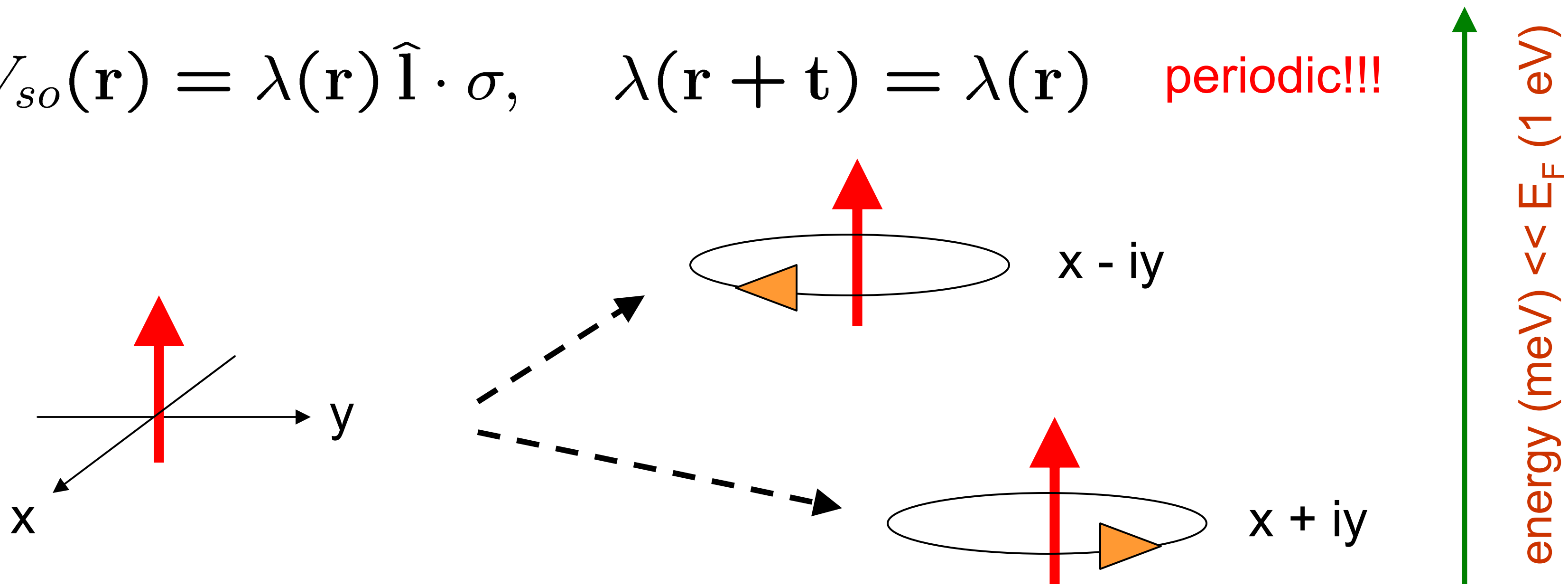


$$V_{so}(\mathbf{r}) = \frac{\hbar}{4m^2c^2} \nabla V_{sc} \times \mathbf{p} \cdot \sigma, \qquad V_{sc}(\mathbf{r}) = \sum_a V\left(\mathbf{r} - \mathbf{R}_a\right)$$

for spherically symmetric ionic potentials,

$$V_{so}(\mathbf{r}) = \lambda(\mathbf{r})\,\hat{\mathbf{l}} \cdot \sigma, \qquad \lambda(\mathbf{r} + \mathbf{t}) = \lambda(\mathbf{r})$$

periodic!!!



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How is the atomic spin-orbit coupling manifested in atomic arrays --- solids?

slides on spin-orbit coupling in solids

intrinsic/extrinsic coupling
Bychkov-Rashba, Dresselhaus
spin-orbit fields

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Time reversal symmetry

$$\begin{aligned} t &\rightarrow -t \\ l &\rightarrow -l \\ \sigma &\rightarrow -\sigma \end{aligned}$$

$$\downarrow$$

$$V_{so} \sim l \cdot \sigma \rightarrow V_{so}$$

SOC preserves time reversal symmetry!

- no net magnetization
- Kramers (spin) degeneracy
- does not beak superconductivity
- leads to spin relaxation

compare to the Zeeman Hamiltonian $H_Z \sim B \cdot \sigma \rightarrow -H_Z$

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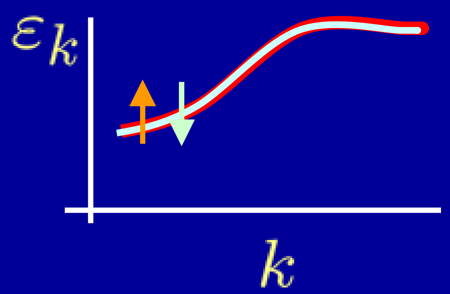
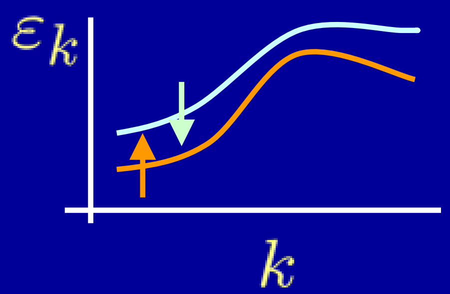
two cases need to be distinguished:

- <u>solids</u> *with* <u>space inversion symmetry</u>



degeneracy

- <u>solids</u> *without* <u>space inversion symmetry</u>



no degeneracy

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Space inversion symmetry

elemental solids (Cu, Al, Si, …)

For a given band n, the following two states have <u>the same</u> energy $\epsilon_{\mathbf{k}n}$

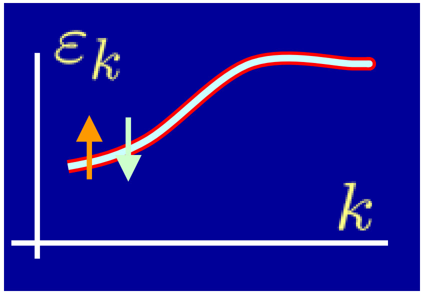
$$\Psi_{\mathbf{k},n\uparrow}(\mathbf{r}) = [a_{\mathbf{k}n}(\mathbf{r})|\uparrow\rangle + b_{\mathbf{k}n}(\mathbf{r})|\downarrow\rangle]\, e^{i\mathbf{k}\cdot\mathbf{r}}$$

$$\Psi_{\mathbf{k},n\downarrow}(\mathbf{r}) = \left[a^*_{-\mathbf{k}n}(\mathbf{r})|\downarrow\rangle - b^*_{-\mathbf{k}n}(\mathbf{r})|\uparrow\rangle\right] e^{i\mathbf{k}\cdot\mathbf{r}}$$

Proof: $$\Psi_{\mathbf{k},n\uparrow}(\mathbf{r}) = [a_{\mathbf{k}n}(\mathbf{r})|\uparrow\rangle + b_{\mathbf{k}n}(\mathbf{r})|\downarrow\rangle]\, e^{i\mathbf{k}\cdot\mathbf{r}}$$

time reversal $\quad -i\sigma_y\widehat{C}$

$$[a^*_{\mathbf{k}n}(\mathbf{r})|\downarrow\rangle - b^*_{\mathbf{k}n}(\mathbf{r})|\uparrow\rangle]\, e^{-i\mathbf{k}\cdot\mathbf{r}}$$



space inversion $\quad \mathbf{k} \to -\mathbf{k}$

$$\left[a^*_{-\mathbf{k}n}(\mathbf{r})|\downarrow\rangle - b^*_{-\mathbf{k}n}(\mathbf{r})|\uparrow\rangle\right] e^{i\mathbf{k}\cdot\mathbf{r}}$$ q.e.d.

One consequence: spin relaxation by momentum scattering (Elliott-Yafet), see later

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Semiconductors (interfaces) without center of inversion

GaAs, InSb, …

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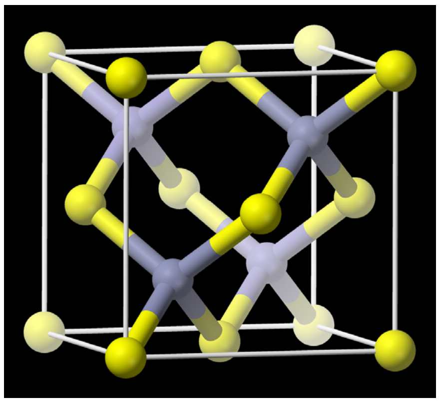
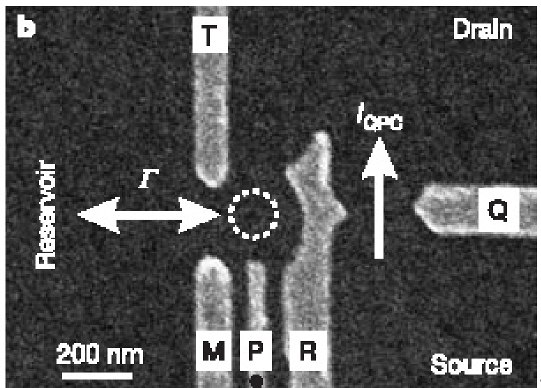
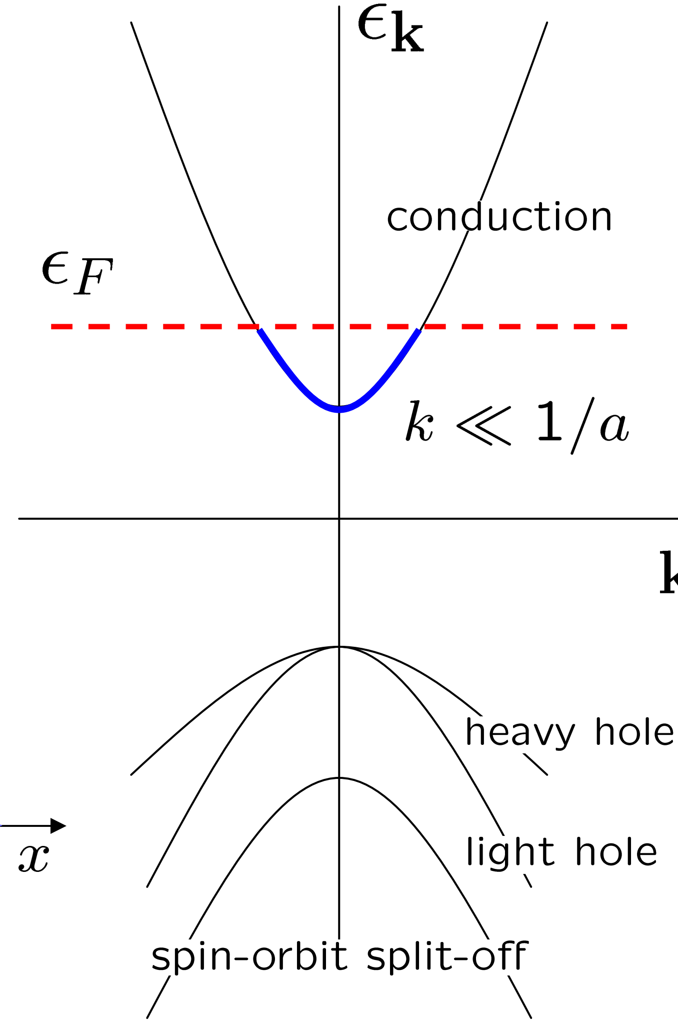
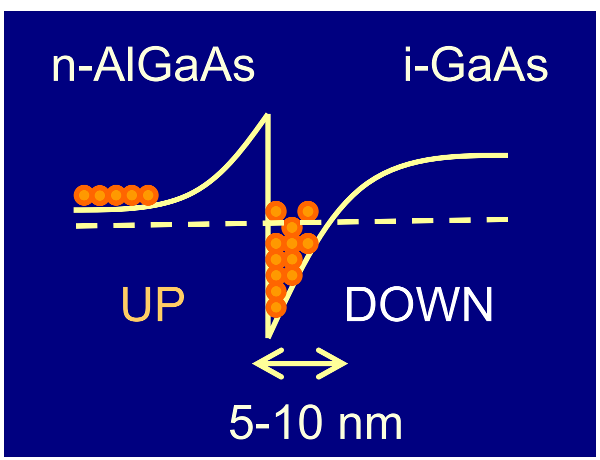
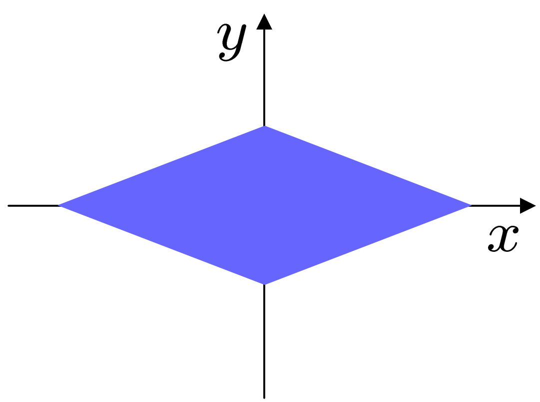




http://qt.tn.tudelft.nl/research/qdots







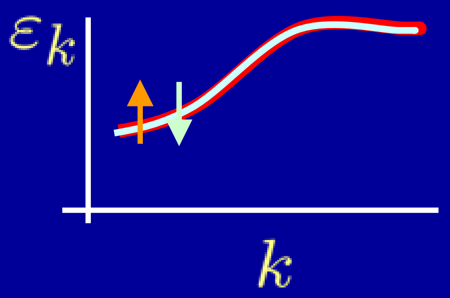
what happens when inversion symmetry is broken?

(GaAs, InSb, interfaces, surfaces, …)

emergence of spin-orbit fields

Time reversal + space inversion symmetry:

$$\varepsilon_{\mathbf{k}\uparrow} = \varepsilon_{\mathbf{k}\downarrow}$$

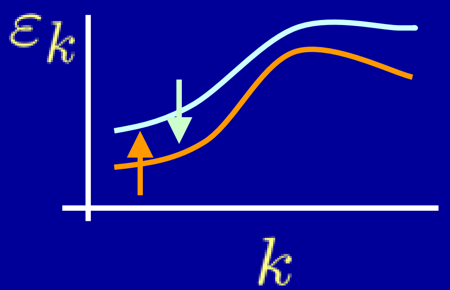


Time reversal symmetry only:

$$\varepsilon_{\mathbf{k}\uparrow} = \varepsilon_{-\mathbf{k}\downarrow}, \quad \varepsilon_{\mathbf{k}\uparrow} \neq \varepsilon_{\mathbf{k}\downarrow}$$

Effective spin-orbit ("magnetic") field Ω:

$$H_1(\mathbf{k}) = \frac{\hbar}{2}\Omega(\mathbf{k}) \cdot \sigma$$



Time reversal symmetry:

$$\Omega(-\mathbf{k}) = -\Omega(\mathbf{k})$$

What are the functional forms and ramifications of the spin-orbit field?

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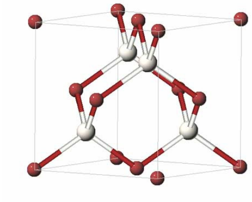
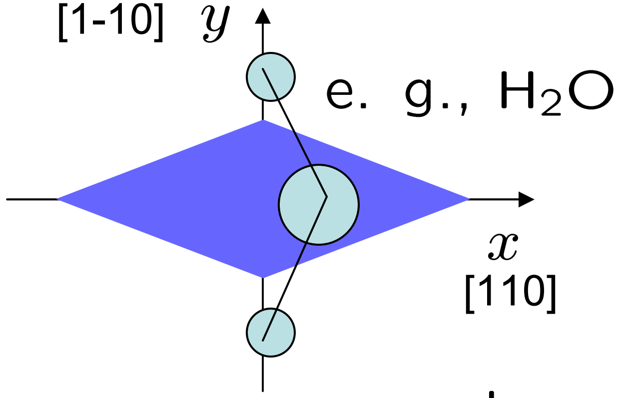
:exploring the symmetry:

a quick path to the effective Hamiltonian





$$C_{2v}: \;\; E,\, C_2,\, \sigma_v(xz),\, \sigma_v(yz)$$

Lowest-order symmetry preserving form:

$$H \sim \left(\alpha x^2 + \beta y^2\right) \times z$$

$$k_x \sim x, \;\; k_y \sim y, \qquad \sigma_x \sim yz, \;\; \sigma_y \sim -xz$$

$$\boxed{H_{so} \sim \alpha\, k_x \sigma_y + \beta\, k_y \sigma_x}$$

Generic linear-k spin-orbit coupling of C_{2v} symmetry

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Deciphering the symmetry:

Bychkov-Rashba and Dresselhaus Hamiltonians

better name: C_{2v} *spin-orbit fields*

$$H_{so} \sim \alpha\, k_x\sigma_y + \beta\, k_y\sigma_x$$

$$H_{so} \sim \frac{1}{2}(\alpha+\beta)(k_x\sigma_y + k_y\sigma_x) + \frac{1}{2}(\alpha-\beta)(k_x\sigma_y - k_y\sigma_x)$$

$$\boxed{H_{so} = \underbrace{\gamma_D(k_x\sigma_y + k_y\sigma_x)}_{D_{2d}\ \text{Dresselhaus}} + \underbrace{\alpha_{BR}(k_x\sigma_y - k_y\sigma_x)}_{C_{4v}\ \text{Bychkov-Rashba}}}$$

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Dresselhaus term

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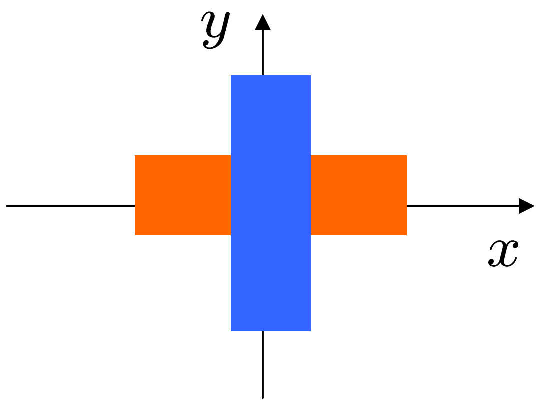
$$\alpha = \beta : \quad \alpha_{BR} = 0, \; \gamma_D = \alpha$$

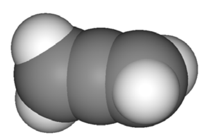
$$H_{so} = H_D = \gamma_D (k_x \sigma_y + k_y \sigma_x)$$

$$H_D \sim \left(x^2 - y^2\right) \times z$$

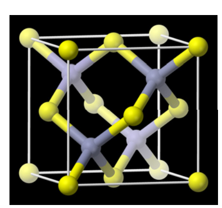


D_{2d}

$E, \; 2S_4, \; C_2, \; 2C_h, \; 2C_2', 2\sigma_d$



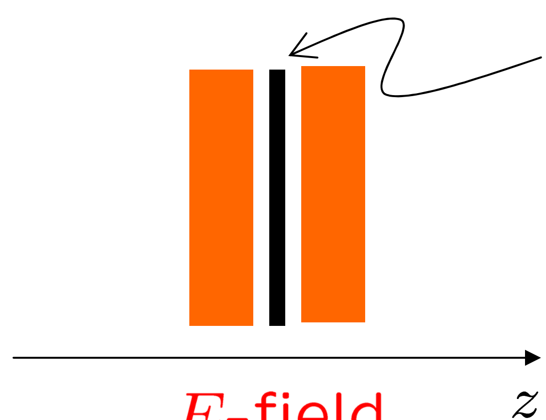
allene



GaAs

bulk-inversion asymmetry

GaAs, ~~Si~~



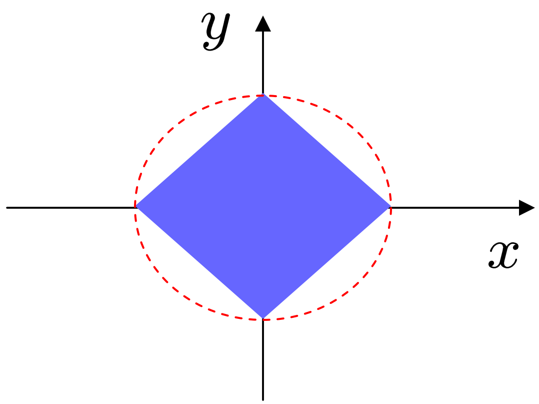
E-field

Bychkov-Rashba term

$$\alpha = -\beta : \quad \alpha_{BR} = \alpha,\ \gamma_D = 0$$

$$H_{so} = H_{BR} = \alpha_{BR}(k_x\sigma_y - k_y\sigma_x)$$

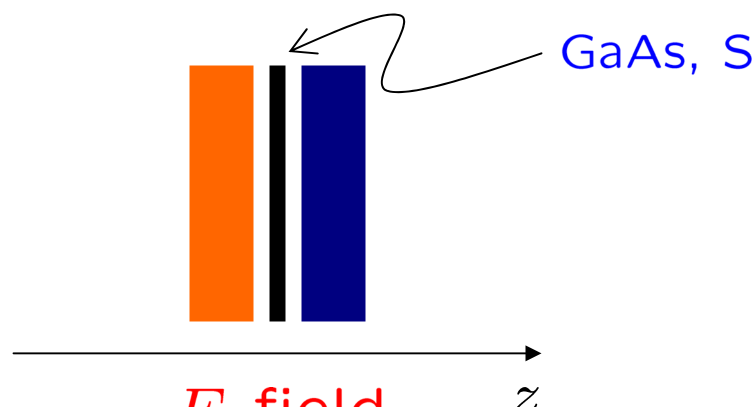
$$H_{BR} \sim \left(x^2 + y^2\right) \times z$$



C_{4v}

E, $2C_4$, C_2, $2\sigma_v$, $2\sigma_d$

structure-inversion asymmetry



E-field

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Dresselhaus and Bychkov-Rashba spin-orbit coupling fields

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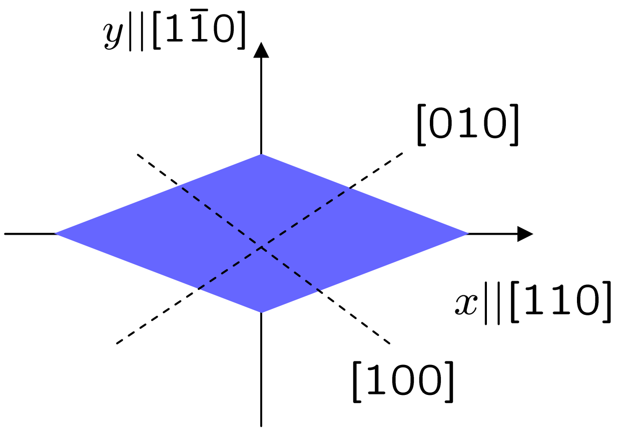
$$H_D = \gamma_D(k_x\sigma_y + k_y\sigma_x) = \mathbf{w}_D \cdot \sigma$$

$$H_{BR} = \alpha_{BR}(k_x\sigma_y - k_y\sigma_x) = \mathbf{w}_{BR} \cdot \sigma$$

$$\mathbf{w}_D = \gamma_D(k_y, k_x)$$

$$\mathbf{w}_{BR} = \alpha_{BR}(-k_y, k_x)$$

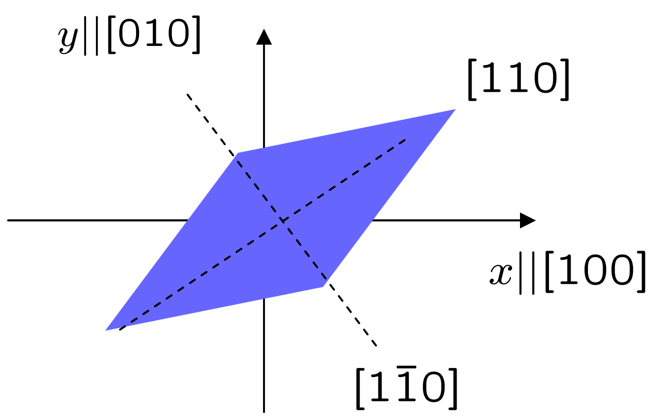


$$H_D = \gamma_D(k_x\sigma_x - k_y\sigma_y)$$

$$H_{BR} = \alpha_{BR}(k_x\sigma_y - k_y\sigma_x)$$

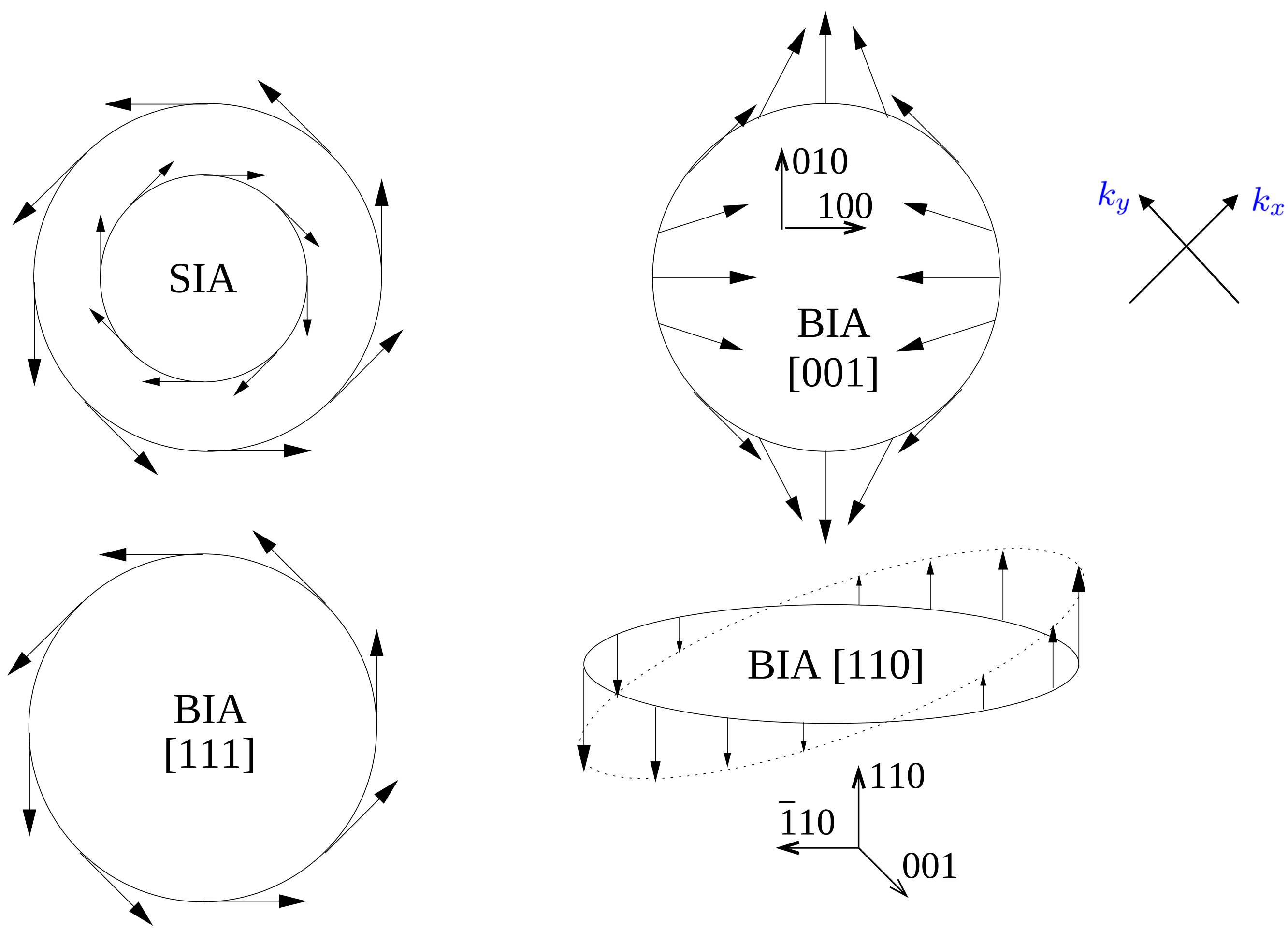
$$\mathbf{w}_D = \gamma_D(k_x, -k_y)$$

$$\mathbf{w}_{BR} = \alpha_{BR}(-k_y, k_x)$$



field vectors

$$\mathbf{w}_{BR} = \gamma_D(-k_y, k_x) \qquad \mathbf{w}_D = \gamma_D(k_y, k_x)$$



From: I. Zutic, J. Fabian, S. Das Sarma, Rev. Mod. Phys. 76, 323 (2004)

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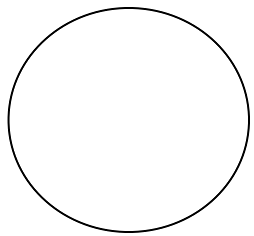
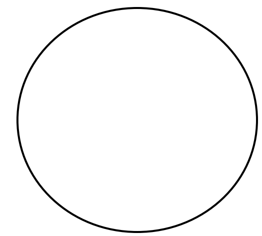
field magnitudes

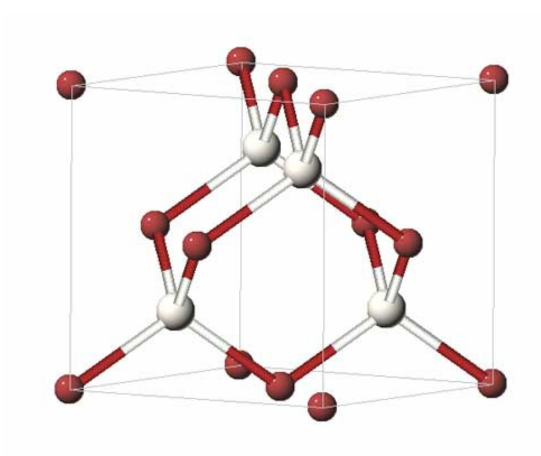
$$|\mathbf{w}_{BR}|^2 = \alpha_{BR}^2(k_x^2 + k_y^2)$$

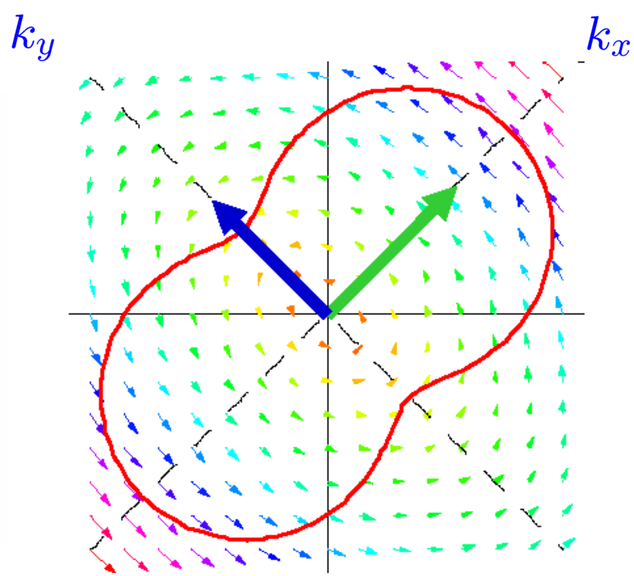
$$|\mathbf{w}_D|^2 = \gamma_D^2(k_x^2 + k_x^2)$$





$$|\mathbf{w}_{BR} + \mathbf{w}_D|^2 = (\alpha_{BR}^2 + \gamma_D^2)(k_x^2 + k_y^2) + 2\alpha_{BR}\gamma_D(k_x^2 - k_y^2)$$





Orientation depends on αγ

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Higher-order terms

M. Gmitra, A. Matos-Abiague, C. Ambrosch-Draxl, and J. Fabian, arXiv:0907.4149

$$H_{so} \sim \alpha(k_x, k_y)\, k_x\sigma_y + \beta(k_x, k_y)\, k_y\sigma_x$$

$$\alpha(k_x, k_y) = \alpha_0 + \alpha^{(11)}k_x^2 + \alpha^{(12)}k_y^2 + \ldots$$

$$\beta(k_x, k_y) = \beta_0 + \beta^{(11)}k_x^2 + \beta^{(12)}k_y^2 + \ldots$$

$$\begin{aligned} H_{BR}^{\mathrm{cub}} &\sim \frac{1}{2}\left[(\alpha^{(11)} - \beta^{(12)})k_x^2 + (\alpha^{(12)} - \beta^{(11)})k_y^2\right] k_x\sigma_y \\ &+ \frac{1}{2}\left[(-\alpha^{(12)} + \beta^{(11)})k_x^2 + (-\alpha^{(11)} + \beta^{(12)})k_y^2\right] k_y\sigma_x \end{aligned}$$

$$\begin{aligned} H_{D}^{\mathrm{cub}} &\sim \frac{1}{2}\left[(\alpha^{(11)} + \beta^{(12)})k_x^2 + (\alpha^{(12)} + \beta^{(11)})k_y^2\right] k_x\sigma_y \\ &+ \frac{1}{2}\left[(\alpha^{(12)} + \beta^{(11)})k_x^2 + (\alpha^{(11)} + \beta^{(12)})k_y^2\right] k_y\sigma_x \end{aligned}$$

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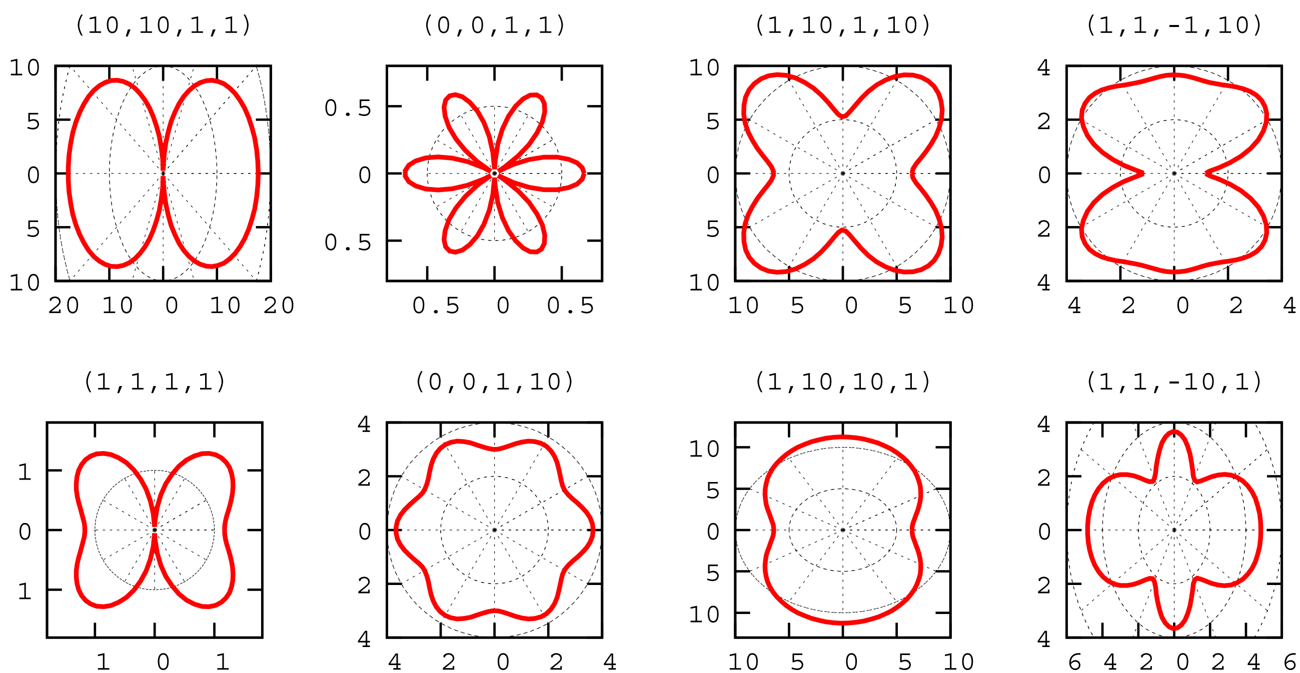
Cubic terms: magnitudes

M. Gmitra, A. Matos-Abiague, C. Ambrosch-Draxl, and J. Fabian, arXiv:0907.4149

$$C_{4v} \quad H_{BR}^{\text{cub}} \sim \left(\alpha_{BR}^{(1)} k_x^2 + \alpha_{BR}^{(2)} k_y^2\right) k_x \sigma_y - \left(\alpha_{BR}^{(2)} k_x^2 + \alpha_{BR}^{(1)} k_y^2\right) k_y \sigma_x$$

$$D_{2d} \quad H_{D}^{\text{cub}} \sim \left(\gamma_{D}^{(1)} k_x^2 + \gamma_{D}^{(2)} k_y^2\right) k_x \sigma_y + \left(\gamma_{D}^{(2)} k_x^2 + \gamma_{D}^{(1)} k_y^2\right) k_y \sigma_x$$



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