Introduction to topology in solids

Jaroslav Hamrle

Charles University, Prague, Czech Republic

hamrle@karlov.mff.cuni.cz

March 8, 2018

Intro

- Berry phase, Berry connection, Berry curvature
- degenerated system, Dirac equation
- Berry curvature and transport
- relation between Berry curvature and Kubo formula
- time reversal operator, Kramers degeneracy
- spin-orbit coupling of light

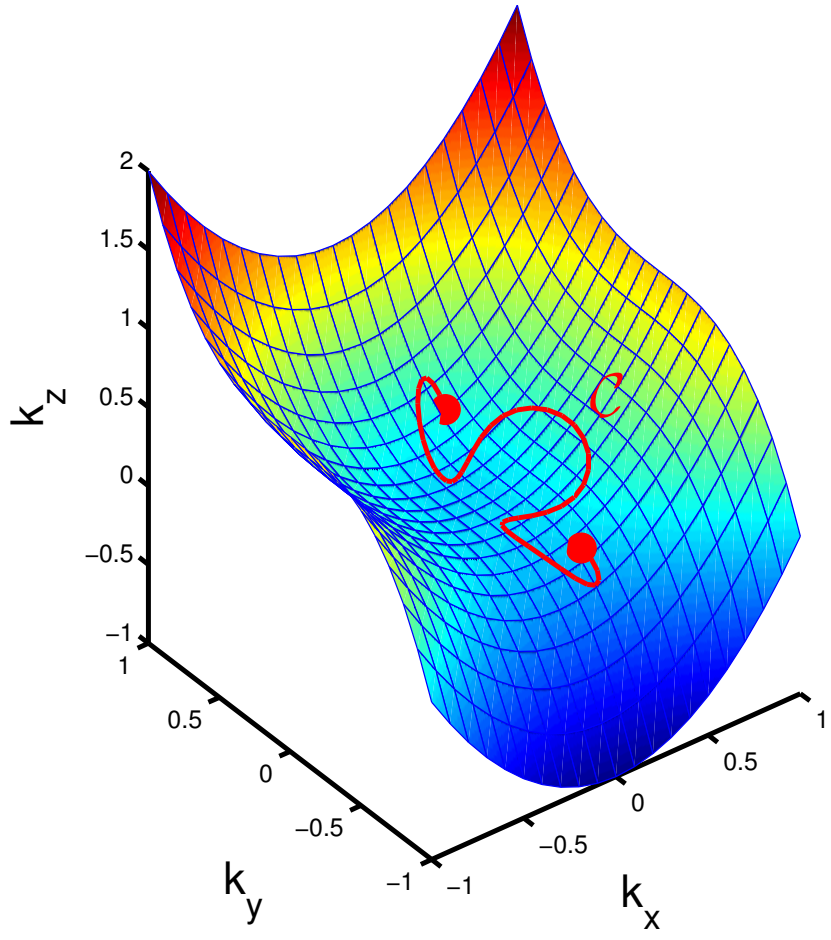
Berry phase, Berry connection, Berry curvature

Phase in parameters space : I

Consider a system described by Hamiltonian depending on time through sets of parametres $\mathcal{R}(t) = (R_1(t), R_2(t), \ldots)$, i.e.

$$H = H(\mathcal{R}(t))$$

- adiabatic evolution of the system as $\mathcal{R}(t)$ moves slowly along a path $\mathcal{C}$ in the parameter space
- parametr space is for example
  - $\rightarrow$ k-space
  - $\rightarrow$ direction of magnetic fied B, etc.



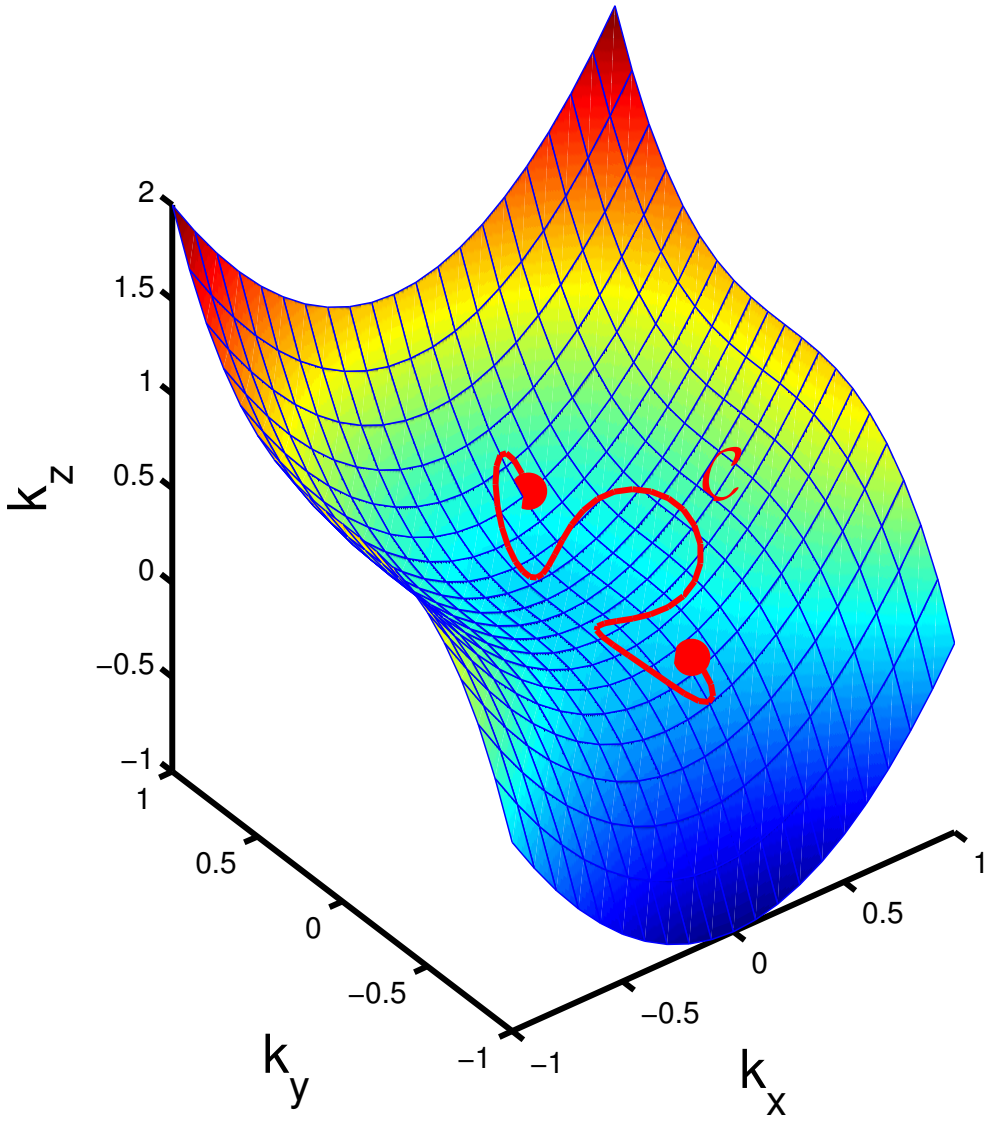
Xiao et al, arxiv:0907.2021 (2009)
Berry (1983)

Phase in parameters space : I

Let us introduce instantaneous orthonormal basis for each $H(\mathcal{R})$

$$H(\mathcal{R})\,|n(\mathcal{R})\rangle = \epsilon_n(\mathcal{R})\,|n(\mathcal{R})\rangle$$

- However, the phase factor of $|n(\mathcal{R})\rangle$ is not determined.
- We require that phase of the basis functions $|n(\mathcal{R})\rangle$ is smooth along path $\mathcal{C}$ in the parameter space.

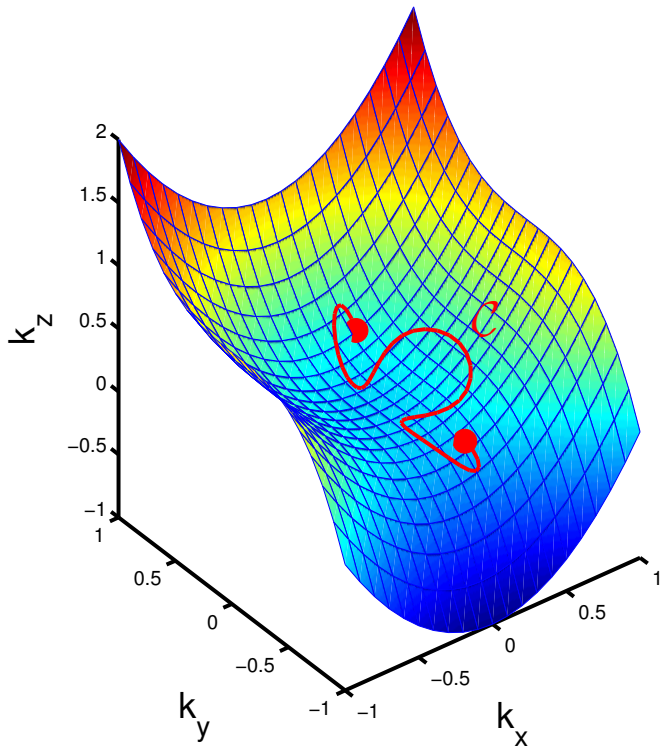


Derivation 1 of Berry connection:

For simplicity, we assume the path $\mathcal{C}$ is on isoenergy surface $\epsilon(\mathcal{R})_n = \epsilon_n = \text{const}_n$. Then, the wavefunction over the path $\mathcal{C}$ is

$$|\psi_n(t)\rangle = e^{i\gamma_n(\mathcal{R}(t))} e^{-\frac{i}{\hbar}\epsilon_n t} |n(\mathcal{R}(t))\rangle$$

where phase consist of phase $\gamma_n(\mathcal{R}(t))$ and dynamic phase $-i\epsilon_n t/\hbar$.



Note:

Generally, when $\epsilon_n(\mathcal{R})$ changes on the path $\mathcal{C}$, the wavefunction becomes

$$|\psi_n(t)\rangle = e^{i\gamma_n(\mathcal{R}(t))} e^{-\frac{i}{\hbar}\int_0^t \mathrm{d}t' \epsilon_n(\mathcal{R}(t'))} |n(\mathcal{R}(t))\rangle$$

where phase consist of phase $\gamma_n(\mathcal{R}(t))$ and dynamical phase factor.

Derivation 1 of Berry connection:

Inserting this wavefunction $|\psi_n(t)\rangle = e^{i\gamma_n(\mathcal{R}(t))} e^{-\frac{i}{\hbar}\epsilon_n t} |n(\mathcal{R}(t))\rangle$ to the Schrodinger equation

$$i\hbar \frac{\partial}{\partial t} |\psi_n(t)\rangle = H(\mathcal{R}(t)) |\psi_n(t)\rangle$$

we got

$$i\frac{\partial \gamma(\mathcal{R})}{\partial \mathcal{R}} |n(\mathcal{R})\rangle + \frac{\partial}{\partial \mathcal{R}} |n(\mathcal{R})\rangle = 0$$

multiplying from left by $\langle n(\mathcal{R})|$

$$\frac{\partial \gamma(\mathcal{R})}{\partial \mathcal{R}} = i \langle n(\mathcal{R})| \frac{\partial}{\partial \mathcal{R}} n(\mathcal{R})\rangle = i\mathcal{A}_n(\mathcal{R})$$

where $\mathcal{A}_n(\mathcal{R})$ is Berry connection or Berry vector potential.

$$\mathcal{A}_n(\mathcal{R}) = i \langle n(\mathcal{R})| \frac{\partial}{\partial \mathcal{R}} |n(\mathcal{R})\rangle$$

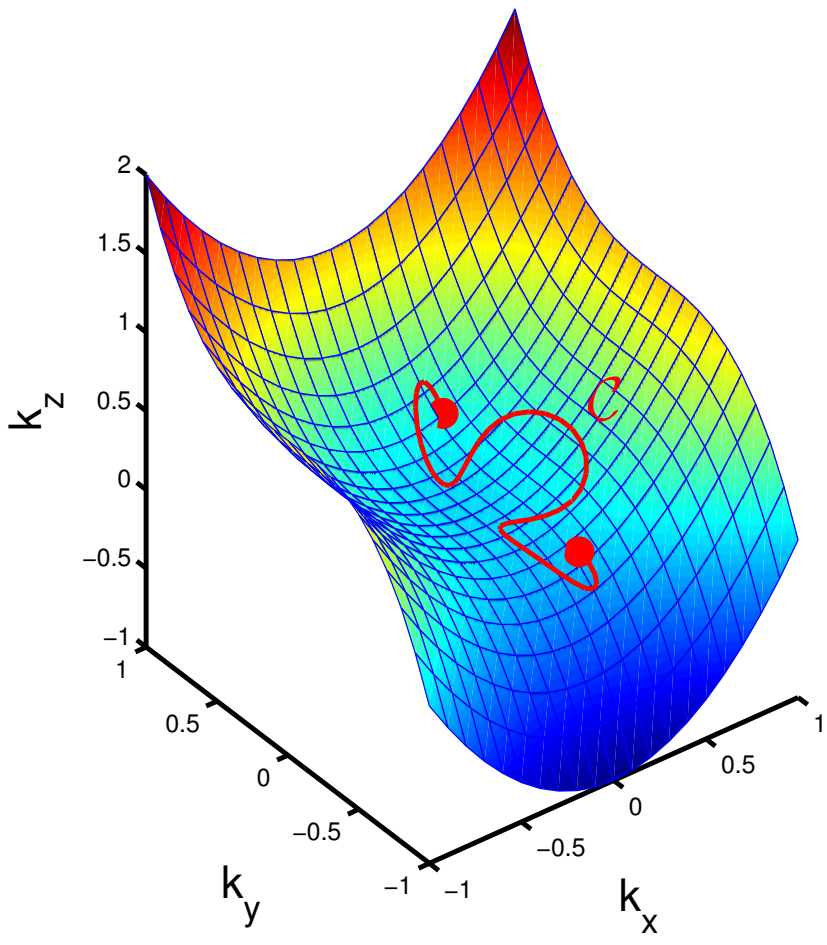
Derivation 1 of Berry connection:

i.e. $\mathcal{A}_n(\mathcal{R})$ expresses speed of change of phase on element of the path,

$$\mathcal{A}_n(\mathcal{R}) = \frac{\partial \gamma_n}{\partial \mathcal{R}} = i \langle n(\mathcal{R}) | \frac{\partial}{\partial \mathcal{R}} | n(\mathcal{R}) \rangle$$

Finally, the change of phase γ_n between starting and final point of path can be expressed as a path integral in the parameter space

$$\gamma_n = \int_{\mathcal{C}} \mathrm{d}\gamma_n = \int_{\mathcal{C}} \mathrm{d}\mathcal{R} \cdot \mathcal{A}_n(\mathcal{R})$$



Derivation 2 of Berry connection:

Two close eigenwavefunctions $|n(\mathcal{R})\rangle$ and $|n(\mathcal{R}+\Delta\mathcal{R})\rangle$ are scalarly multiplied:

$$\langle n(\mathcal{R})|n(\mathcal{R}+\Delta\mathcal{R})\rangle \approx 1+\Delta\mathcal{R}\,\langle n(\mathcal{R})|\nabla_{\mathcal{R}}|n(\mathcal{R})\rangle$$
$$\approx \exp[-i\Delta\mathcal{R}\cdot\mathcal{A}_n(\mathcal{R})] = \exp[-i\gamma_n] = \exp[-i[\gamma_n(\mathcal{R}+\Delta\mathcal{R})-\gamma_n(\mathcal{R})]]$$

where Berry connection $\mathcal{A}_n(\mathcal{R})$ is

$$\mathcal{A}_n(\mathcal{R}) = i\,\langle n(\mathcal{R})|\nabla_{\mathcal{R}}|n(\mathcal{R})\rangle$$

and Berry phase γ_n is expressed again as

$$\gamma_n = \int_{\mathcal{C}} \mathrm{d}\gamma_n = \int_{\mathcal{C}} \mathrm{d}\mathcal{R}\cdot\mathcal{A}_n(\mathcal{R})$$

Weng et al, arxiv:1508.02967 (2015)

Berry connection: gauge transformation

Obviously, Berry connection $\mathcal{A}_n(\mathcal{R})$ is gauge-dependent. We introduce gauge by applying

$$|n'(\mathcal{R})\rangle \to e^{i\zeta(\mathcal{R})}\,|n(\mathcal{R})\rangle$$

where $\zeta(\mathcal{R})$ is arbitrary smooth function. Then $\mathcal{A}_n(\mathcal{R})$ transforms as

$$\begin{aligned}\mathcal{A}'_n(\mathcal{R}) \to \langle n'(\mathcal{R})|\frac{\partial}{\partial\mathcal{R}}|n'(\mathcal{R})\rangle &= i\,\langle ne^{-i\zeta}|\frac{\partial}{\partial\mathcal{R}}|e^{i\zeta}n\rangle \\ &= i\,\langle ne^{-i\zeta}|\left[e^{i\zeta}\,|\frac{\partial}{\partial\mathcal{R}}n\rangle + i\,|e^{i\zeta}n\rangle\,\frac{\partial\zeta}{\partial\mathcal{R}}\right] \\ &= \mathcal{A}_n(\mathcal{R}) - \frac{\partial}{\partial\mathcal{R}}\zeta(\mathcal{R})\end{aligned}$$

Consequently, phase γ_n between starting and final points changes by $\zeta(\mathcal{R}(0)) - \zeta(\mathcal{R}(T))$ where $\mathcal{R}(0)$ and $\mathcal{R}(T)$ are initial and final points of the path $\mathcal{C}$.

Berry connection: gauge transformation in Maxwell equations

$$\mathcal{A}'_n(\mathcal{R}) = \mathcal{A}_n(\mathcal{R}) - \frac{\partial}{\partial \mathcal{R}}\zeta(\mathcal{R})$$

Note analogy with gauge transformation in Maxwell equations:

$$\mathbf{B} = \nabla \times \mathbf{A}, \qquad \mathbf{E} = -\nabla\varphi - \frac{\partial}{\partial t}\mathbf{A}$$

where $\mathbf{A}$ and φ are magentic vector potential and electric potentials.

Gauge transformation of $\mathbf{A}$ and φ by arbitrary scalar function $\Psi(\mathbf{r}, t)$ (called gauge function)

$$\mathbf{A'} \to \mathbf{A} + \nabla\Psi, \qquad \varphi' \to \varphi - \frac{\partial \Psi}{\partial t}$$

Under this transformation, the $\mathbf{E}$ and $\mathbf{B}$ do not change. Note, we assume the gauge phase $\zeta(\mathcal{R})$ does not depend on time.

https://en.wikipedia.org/wiki/Gauge_fixing

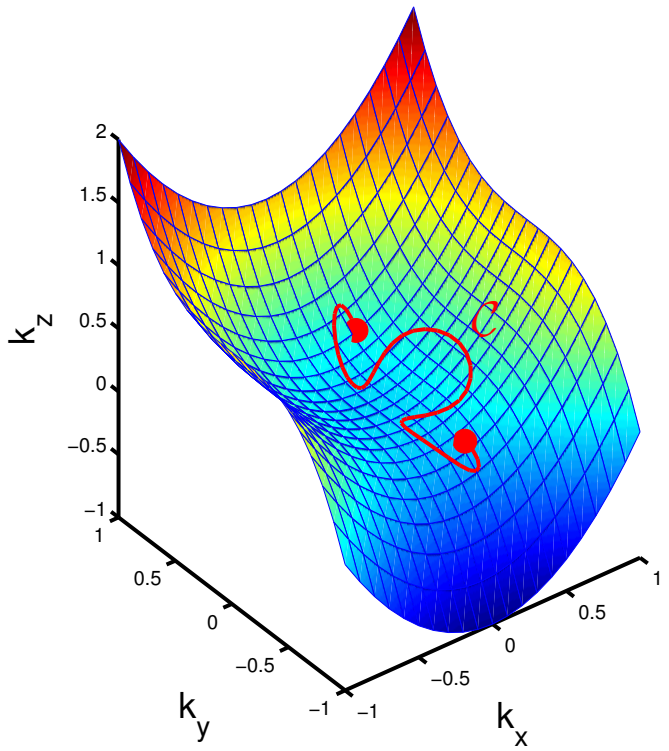
Berry connection: gauge transformation

$$|n'(\mathcal{R})\rangle \to e^{i\zeta(\mathcal{R})}\,|n(\mathcal{R})\rangle$$

$$\gamma_n = \int_{\mathcal{C}} \mathrm{d}\mathcal{R}\cdot\mathcal{A}_n(\mathcal{R})$$

Fock 1928: one can always find suitable gauge $\zeta(\mathcal{R})$ so that accumulated phase γ_n along any path $\mathcal{C}$ is always zero

$\Rightarrow$ γ_n was thought to be unimportant and was usually neglected



Berry phase and Berry connection: gauge transformation

Berry 1984:

path $\mathcal{C}$ is closed, i.e. $\mathcal{R}(0) = \mathcal{R}(T)$

$\Rightarrow$ We assume gauge $\exp[i\zeta(\mathcal{R})]$ to be single-valued.

$\Rightarrow$ the gauge must fullfils

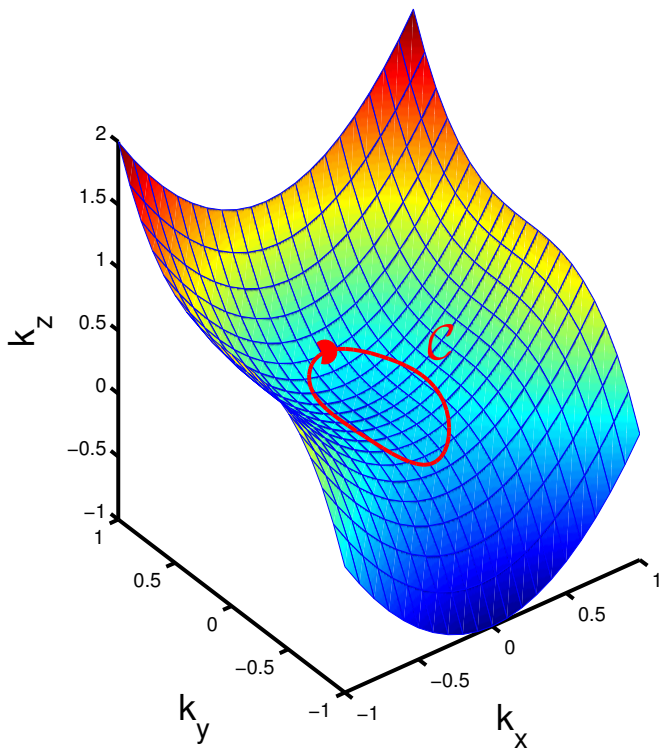
$$\zeta(\mathcal{R}(0)) - \zeta(\mathcal{R}(T)) = 2\pi N$$

N is integer.

$\Rightarrow$ Integral of phase over close path is well-defined, and gauge-invariant (with exception $2\pi N$)

$$\gamma_n = \oint_{\mathcal{C}} \mathrm{d}\mathcal{R} \cdot \mathcal{A}_n(\mathcal{R}) + 2\pi N$$

being known as Berry phase or geometrical phase.



Berry curvature I

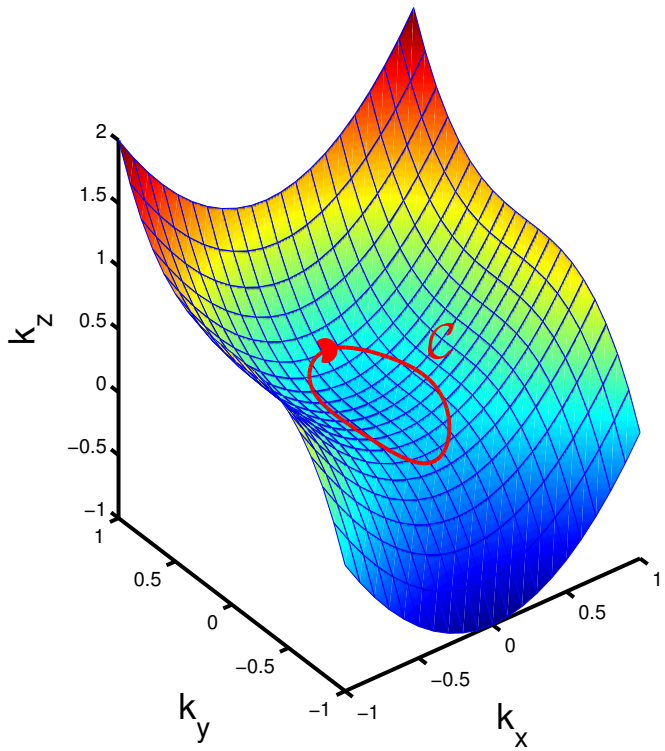
In following, we limit to 3D space of parameters $\mathcal{R}$. In case $\mathcal{R}$ is in 3D, Stokes thorem relates Berry phase as

$$\gamma_n = \oint_{\mathcal{C}} \mathrm{d}\mathcal{R} \cdot \mathcal{A}_n(\mathcal{R}) = \int_S \mathbf{\Omega}_n(\mathcal{R}) \cdot \mathrm{d}S$$

where $\mathbf{\Omega}_n(\mathcal{R})$ is called Berry curvature:

$$\mathbf{\Omega}_n(\mathcal{R}) = \nabla_{\mathcal{R}} \times \mathcal{A}_n(\mathcal{R}) = i \langle \frac{\partial}{\partial R} n| \times |\frac{\partial}{\partial R} n\rangle$$

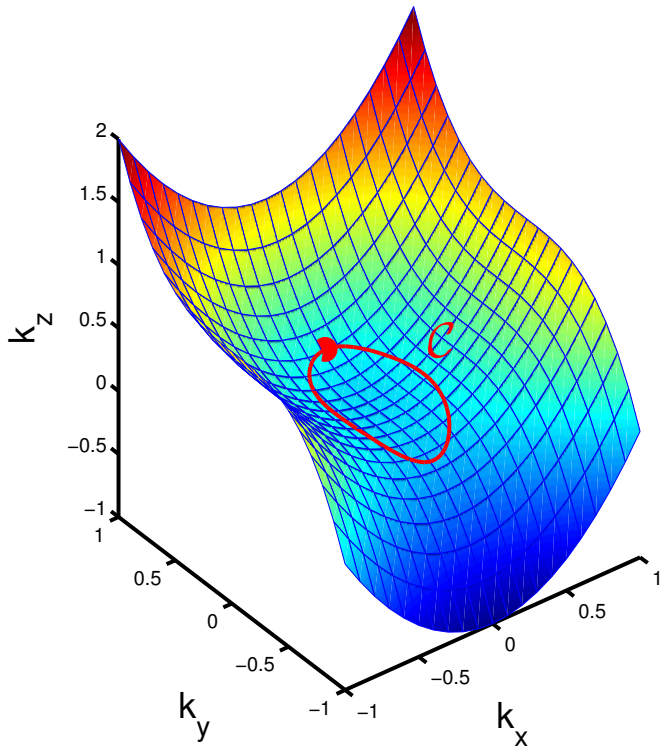
- $\mathbf{\Omega}_n$ is defined for each point of $\mathcal{R}$-space, it is property of each point
- $\mathbf{\Omega}_n$ is gauge invariant (i.e. well-defined, measureble)



Berry curvature in **k**-space

In solid state physics, parameter space $\mathcal{R}$ is **k**-space, i.e. $\mathcal{R} \equiv \mathbf{k}$. Then, Berry curvature in **k**-space:

$$\mathbf{\Omega}_n(\mathbf{k}) = \nabla_{\mathbf{k}} \times \mathcal{A}_n(\mathbf{k}) = i \langle \frac{\partial}{\partial \mathbf{k}} n| \times |\frac{\partial}{\partial \mathbf{k}} n\rangle$$



- Notice that Berry curvature writes in form 'gradient vector-times gradient', which is zero for scalar functions, $\nabla\psi \times \nabla\psi = 0$
- Here, there is gradient in bra and ket wavefunctions, $\langle \nabla n| \times |\nabla n\rangle \neq 0$, as $\langle \nabla n|$ and $|\nabla n\rangle$ differ by phase.

Berry curvature and transport

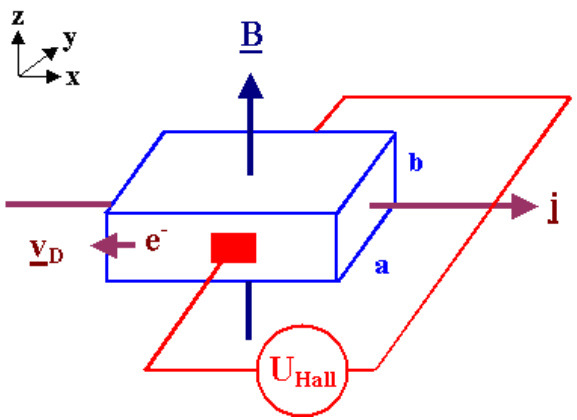
$\mathbf{\Omega}_n$ can be viewed as the magnetic field in the **k**-space

$$\dot{\mathbf{k}} = -\frac{e}{\hbar}\left(\mathbf{E} + \dot{\mathbf{r}} \times \mathbf{B}\right)$$

$$\dot{\mathbf{r}} = \frac{1}{\hbar}\frac{\partial \epsilon_n(\mathbf{k})}{\partial \mathbf{k}} - \dot{\mathbf{k}} \times \mathbf{\Omega}_n(\mathbf{k})$$

$\Rightarrow$ non-zero Berry curvature is responsible for phenomena in solids, where motion is perpendicular to the applied force

- Anomalous (Hall) efffects, spin-Hall effect, $\mathbf{j} = \sigma_{\mathrm{Hall}}\, \mathbf{M} \times \mathbf{E}$
- Nerst effect, spin Nerst effect, $\mathbf{j} = N\, \mathbf{M} \times \boldsymbol{\nabla} \mathbf{T}$
- magneto-optical Kerr effect, magnetic circular dichroism: off-diagonal permittivity $\epsilon_{xy} \neq 0$



Berry curvature: symmetry considarations

Inversion (point) symmetry:

Inversion symmetry is given by symmtery of the Hamiltonian

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

leading to symmetry in eigenstates and eigenvalues:

$$\epsilon_n(\mathbf{k}) = \epsilon_n(-\mathbf{k}), \qquad u_n(\mathbf{k}) = u_n(-\mathbf{k})$$

Then, following definition of $\mathbf{\Omega}_n(\mathbf{k}) = i\,\langle \frac{\partial}{\partial \mathbf{k}} n| \times |\frac{\partial}{\partial \mathbf{k}} n\rangle$

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

Time reversal symmetry:

Under time reversal: $\mathbf{\Omega}_n(\mathbf{k}) = -\mathbf{\Omega}_n(-\mathbf{k})$

$\Rightarrow \Omega \neq 0$ only when time or inversion symmetry is broken

Two level degenerate system

Two level degenerate system: Hamiltonian

Let us have two-fold degenerate states $|a\rangle$, $|b\rangle$

$$H_0 |a\rangle = \epsilon_0 |a\rangle$$
$$H_0 |b\rangle = \epsilon_0 |b\rangle$$

Adding perturbation Hamiltonian ΔH, we search for solution $|u\rangle$

$$(H + \Delta H) |u\rangle = \epsilon |u\rangle$$

Assuming the solution is in basis of original wavefunctions, $|u\rangle = a |a\rangle + b |b\rangle$, the general form of two-level perturbation Hamiltionan is as (i) H must be Hermitian, $H = H^*$ (ii) without lost of generality, we assume degenerate eigenfrequencies are zeros ($\epsilon_0 = 0$).

$$\Delta H(\mathcal{R}) = \begin{bmatrix} Z & X + iY \\ X - iY & -Z \end{bmatrix} = \begin{bmatrix} Z & R_+ \\ R_- & -Z \end{bmatrix}$$

Two level degenerate system: Hamiltonian

$$\Delta H(\mathcal{R}) = \begin{bmatrix} Z & X+iY \\ X-iY & -Z \end{bmatrix} = \begin{bmatrix} Z & R_+ \\ R_- & -Z \end{bmatrix}$$

where $X(\mathcal{R})$, $Y(\mathcal{R})$, $Z(\mathcal{R})$ depends on path in the parameter space $\mathcal{R}$. Schrodinger equation has eigenvector $|u\rangle = a|a\rangle + b|b\rangle$

$$\begin{bmatrix} Z & R_+ \\ R_- & -Z \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = \epsilon \begin{bmatrix} a \\ b \end{bmatrix}$$

leading to two solutions $+$, $-$

$$\epsilon_\pm = \epsilon_0 \pm \sqrt{X^2+Y^2+Z^2} = \pm R$$

$$|\pm\rangle \equiv |u_\pm\rangle = a_\pm |a\rangle + b_\pm |b\rangle$$

$$\left(\frac{b}{a}\right)_\pm = -\frac{Z-\epsilon_\pm}{X+iY} = \frac{X-iY}{Z+\epsilon_\pm}$$

Two distinct meaning of Pauli matrices

$$\tilde{\sigma}_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \qquad \tilde{\sigma}_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \qquad \tilde{\sigma}_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

1. Pauli matrices as a spin operator **S** in up-down bases of the spin part of the wavefunction,

$$\chi = \begin{bmatrix} u_\uparrow \\ u_\downarrow \end{bmatrix}$$

The Hamiltonian of spin in magnetic field is (Zeeman term)

$$H = -\boldsymbol{\mu} \cdot \mathbf{B} = \frac{e}{mc} \mathbf{S} \cdot \mathbf{B}, \qquad \mathbf{S} = \frac{\hbar}{2} \boldsymbol{\sigma} = \frac{\hbar}{2} \begin{bmatrix} \sigma_x \\ \sigma_y \\ \sigma_z \end{bmatrix}$$

Comment: $\boldsymbol{\sigma}$ denotes *vector* of Pauli matrices.

Two distinct meaning of Pauli matrices

$$\tilde{\sigma}_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \qquad \tilde{\sigma}_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \qquad \tilde{\sigma}_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

2. Pauli matrices as generating matrices of any Hermitian 2x2 matrix. I.e. they are generating (base) matrices of any two-level system

$$\Delta H(\mathcal{R}) = \begin{bmatrix} Z & X + iY \\ X - iY & -Z \end{bmatrix} = X\sigma_x + Y\sigma_y + Z\sigma_z = \mathbf{h} \cdot \boldsymbol{\sigma}$$

→ 'spin-in-magnetic-field' problem is example of the two level degenerate problems.

→ appearance of σ matrices in two-level degenerate problem may be confusing, suggesting that problem handles spin.

→ two level degenerate system is a very common problem, e.g. spin-orbit coupling, graphene etc.

Two level degenerate system: spin in magnetic field

Free electron under magnetic field has perturbation Hamiltonian

$$\Delta H = -\boldsymbol{\mu} \cdot \mathbf{B} = \frac{e}{mc}\mathbf{S} \cdot \mathbf{B} = \frac{e}{mc}\left[S_x B_x + S_y B_y + S_z B_z\right]$$

where $\boldsymbol{\mu}$, $\mathbf{S}$ are electron's operators of magnetic moment and spin angular momentum, respectively. The spin operators are

$$S_x = \frac{\hbar}{2}\sigma_x \qquad S_y = \frac{\hbar}{2}\sigma_y \qquad S_z = \frac{\hbar}{2}\sigma_z$$

where in basis of up/down spins, the $\sigma_{x/y/z}$ are Pauli matrices:

$$\tilde{\sigma}_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \qquad \tilde{\sigma}_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \qquad \tilde{\sigma}_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

Two level degenerate system: spin in magnetic field

Then, normalized Hamiltonian in up/down spin basis writes:

$$\Delta H \frac{2mc}{e\hbar} = B_x \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} + B_y \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} + B_z \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

$$\Delta H \frac{2mc}{e\hbar} = \begin{bmatrix} B_z & B_x + iB_y \\ B_x - iB_y & -B_z \end{bmatrix}$$

i.e. it has form of general two-level perturbation form as discussed above.

Two level degenerate system: spin in magnetic field

Solving problem, where size/direction of external field is a path parameter, $\mathcal{R} = \frac{e\hbar}{2mc}\mathbf{B}$. Then, Berry curvature is

$$\boldsymbol{\Omega}_+ = i\frac{\langle +|\boldsymbol{\nabla}_{\boldsymbol{\mathcal{R}}} H|-\rangle \times \langle -|\boldsymbol{\nabla}_{\boldsymbol{\mathcal{R}}} H|+\rangle}{(\epsilon_+ - \epsilon_-)^2}$$

where $\nabla_{\boldsymbol{\mathcal{R}}} H$ is vector of σ matrices, namely $\partial H/\partial x = \sigma_x$, $\partial H/\partial y = \sigma_y$, $\partial H/\partial z = \sigma_z$.

Rotating coordinate system that $\mathbf{B} \parallel z$, Berry curvature $\boldsymbol{\Omega}_+$ is

$$\Omega_{+,x} = i\langle +|\sigma_y|-\rangle\langle -|\sigma_z|+\rangle/2R^2 = 0$$

$$\Omega_{+,y} = i\langle +|\sigma_z|-\rangle\langle -|\sigma_x|+\rangle/2R^2 = 0$$

$$\Omega_{+,z} = i\langle +|\sigma_x|-\rangle\langle -|\sigma_y|+\rangle/2R^2 = \frac{1}{2R^2}$$

Rotating coordinate system back,

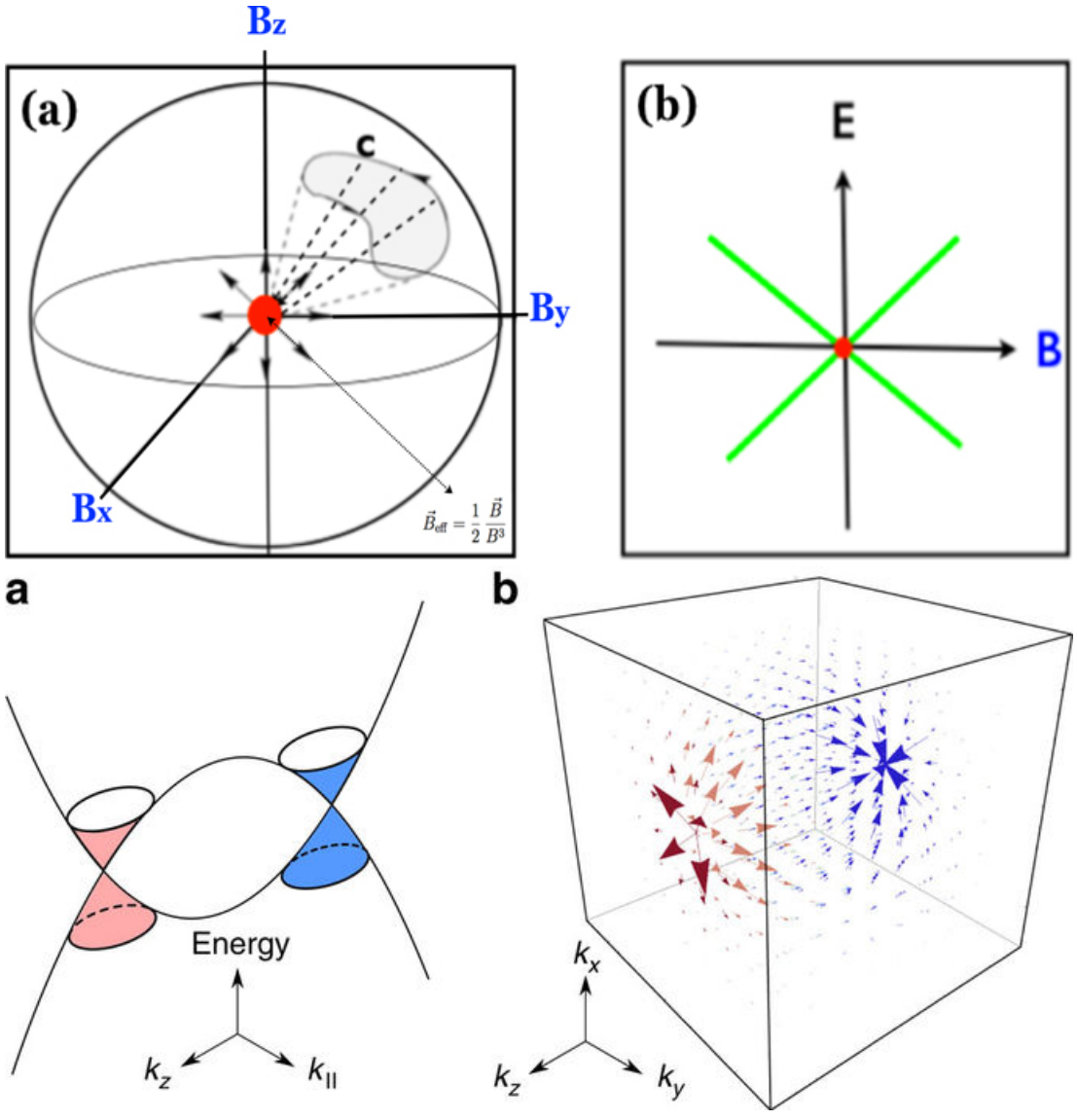
$$\boldsymbol{\Omega}_\pm(\boldsymbol{\mathcal{R}}) = \pm\frac{\boldsymbol{\mathcal{R}}}{2R^3} = 2\left(\frac{mc}{e\hbar}\right)^2\frac{\mathbf{B}}{B^3}$$

Two level degenerate system: Chern charge

$$\boldsymbol{\Omega}_+(\boldsymbol{\mathcal{R}}) = \frac{\boldsymbol{\mathcal{R}}}{2R^3} \sim \frac{\mathbf{B}}{B^3}$$

$\Rightarrow$ Berry curvature of two-level degenerate state behaves as originating from monopole source with strength $\frac{1}{2}$ located at point of degeneracy, at position $\boldsymbol{\mathcal{R}} = 0$

$\Rightarrow$ degeneracy points serve as a source or drain of Berry curvature flux.

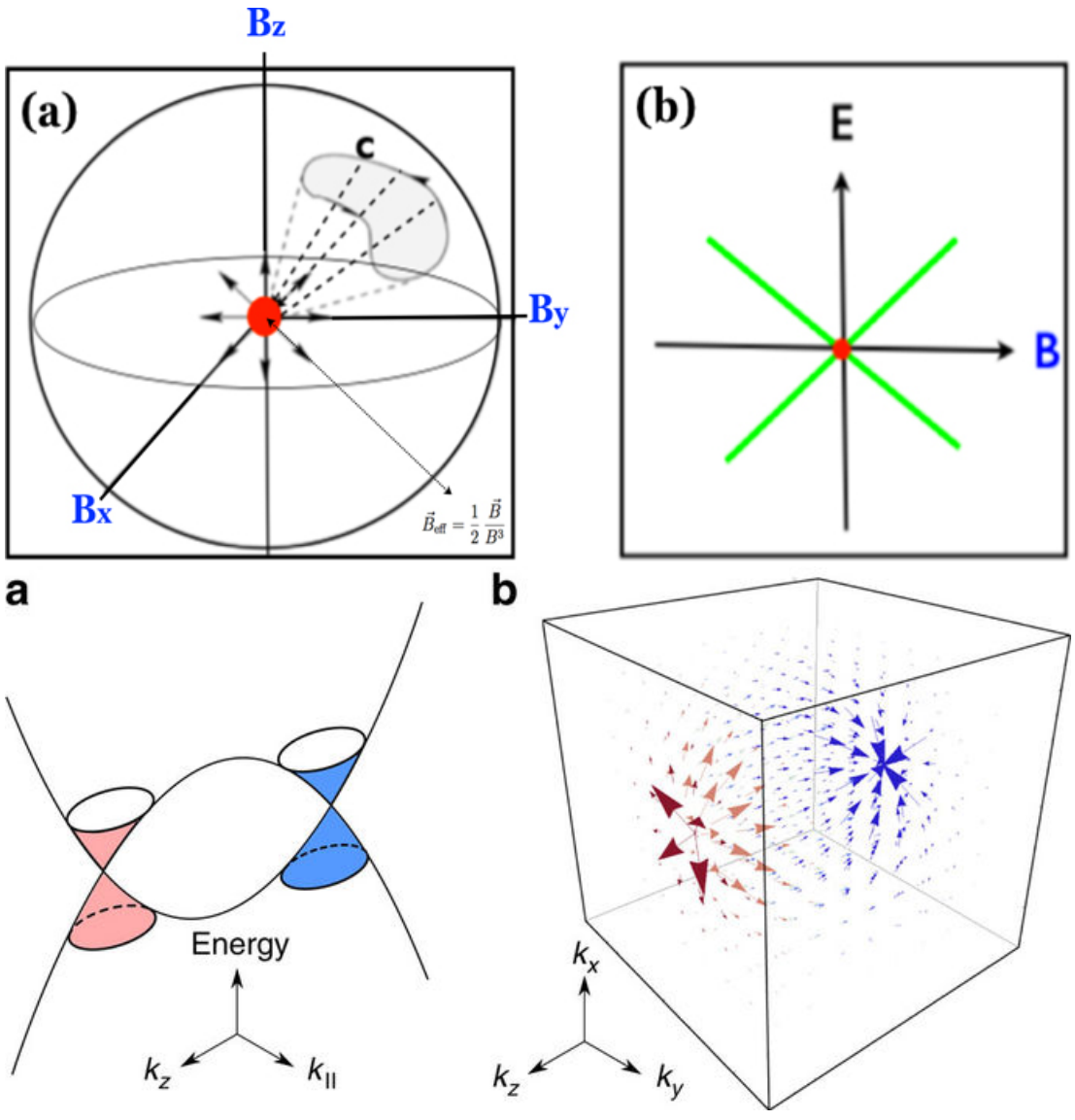


Two level degenerate system: Chern charge

Total flux of Berry curvature by close surface around this degeneracy point is

$$\frac{2}{4\pi}\oint_S \mathbf{\Omega}\cdot \mathrm{d}\mathbf{S} = N,$$

where N=integer, being called Chern charge, enclosed within the area S. Quantized nature of Chern charge is responsible of quantization of many phenomena (e.g. quantum Hall effect)

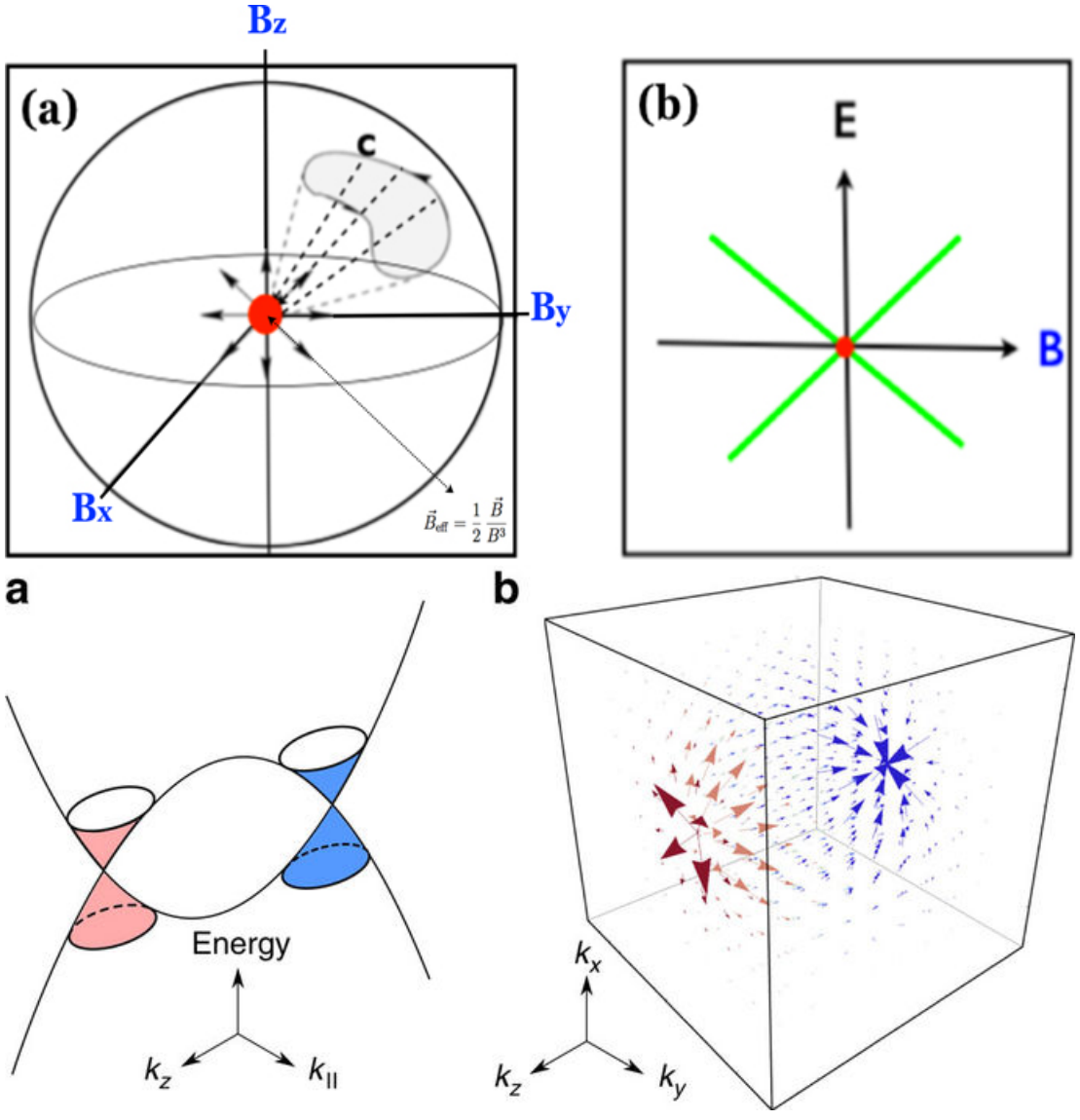


Two level degenerate system: Chern charge

The Berry phase (a.k.a geometrical phase) associated with close path C in the vicinity of the monopole of strength 1/2

$$\gamma_C = \int_S \mathbf{\Omega} \cdot \mathrm{d}\mathbf{S}$$

$$= \frac{1}{2}\,(\text{Solid angle given by } \mathbf{S})$$



Two level degenerate system: symmetry

Let as assume, in point $\mathcal{R}_0$, two-level system become degenerate, $\epsilon_n \approx \epsilon_m$

- Then, Berry curvatures $\mathbf{\Omega}_m$, $\mathbf{\Omega}_n$ in the vicinity of $\mathcal{R}_0$ is dominantly determined by (nearly) degenerate states $|n\rangle$, $|m\rangle$ and having opposite signs

$$\mathbf{\Omega}_n = -\mathbf{\Omega}_m = i\frac{\langle n|\boldsymbol{\nabla}_{\mathbf{R}}H|m\rangle \times \langle m|\boldsymbol{\nabla}_{\mathbf{R}}H|n\rangle}{(\epsilon_n - \epsilon_m)^2}$$

- Hence, the change of phase in path around degenerate point $\mathcal{R}_0$ are opposite, $\gamma_{n,C} = -\gamma_{m,C}$.

Dispersion relation of free the electron

- Newton (classical):

$$E = \frac{1}{2}mv^2 = \frac{p^2}{2m}$$

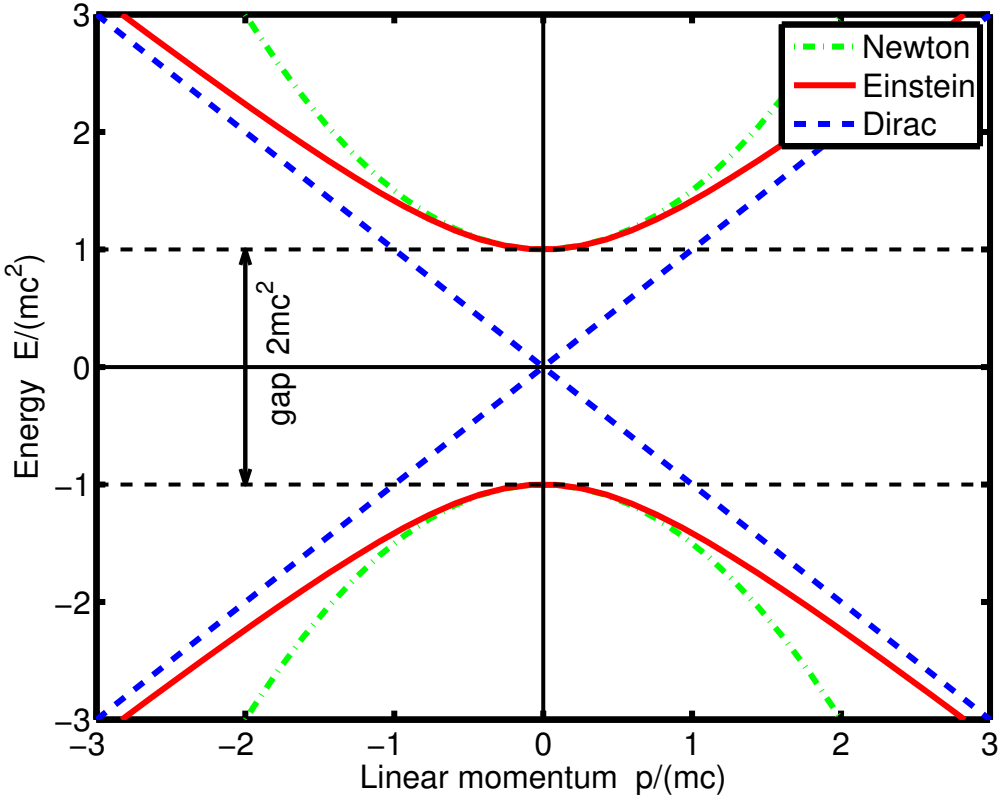
- Einstein (special relativity):

$$E = \sqrt{p^2c^2 + (mc^2)^2}$$

$$\approx mc^2 + \frac{p^2}{2m}$$

- Dirac equation:

$$E = cp$$

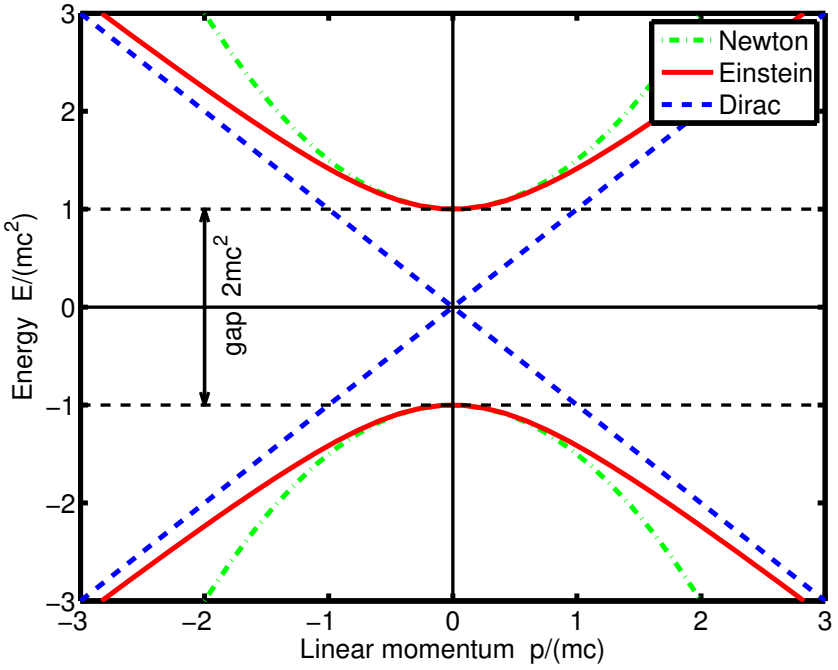


Two level degenerate system: Dirac equation

Dirac equation, describing spin-$\frac{1}{2}$ particle (e.g. electron):

$$\begin{bmatrix} mc^2 & c\boldsymbol{\sigma}\cdot\mathbf{p} \\ c\boldsymbol{\sigma}\cdot\mathbf{p} & -mc^2 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \end{bmatrix} = \epsilon \begin{bmatrix} u_1 \\ u_2 \end{bmatrix}$$

$$u_1 = \begin{bmatrix} u_{1\uparrow} \\ u_{1\downarrow} \end{bmatrix} \qquad u_2 = \begin{bmatrix} u_{2\uparrow} \\ u_{2\downarrow} \end{bmatrix}$$



- u_1, u_2: each two-component wavefunctions (up/down spin)
- u_1, u_2: solution for particle ($m > 0$) and antiparticle ($m < 0$)
- for $\mathbf{p} = 0$, gap $2mc^2$ between particles and antiparticles

Two level degenerate system: effect of mass

→ **Effect of the diagonal term (mass)**

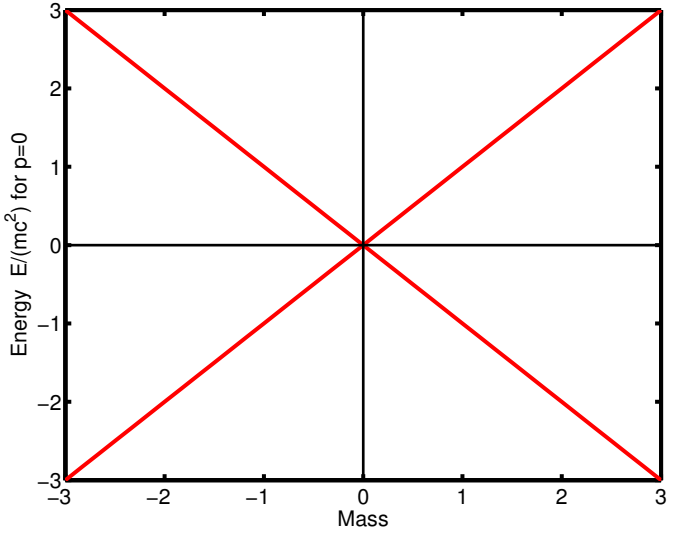
Here, we keep $\mathbf{p} = 0$

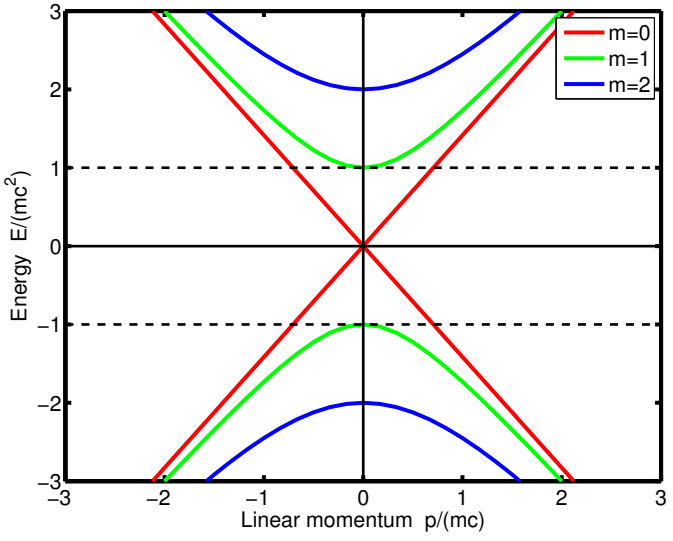
$$H_z = \begin{bmatrix} mc^2 & 0 \\ 0 & -mc^2 \end{bmatrix}$$

→ **Effect of the off-diagonal terms (momentum)**

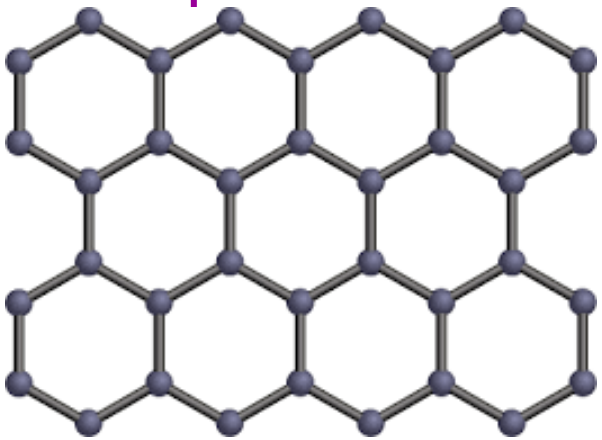
$$H_x = \begin{bmatrix} mc^2 & cp \\ cp & -mc^2 \end{bmatrix}$$

$$H_y = \begin{bmatrix} mc^2 & -icp \\ icp & -mc^2 \end{bmatrix}$$



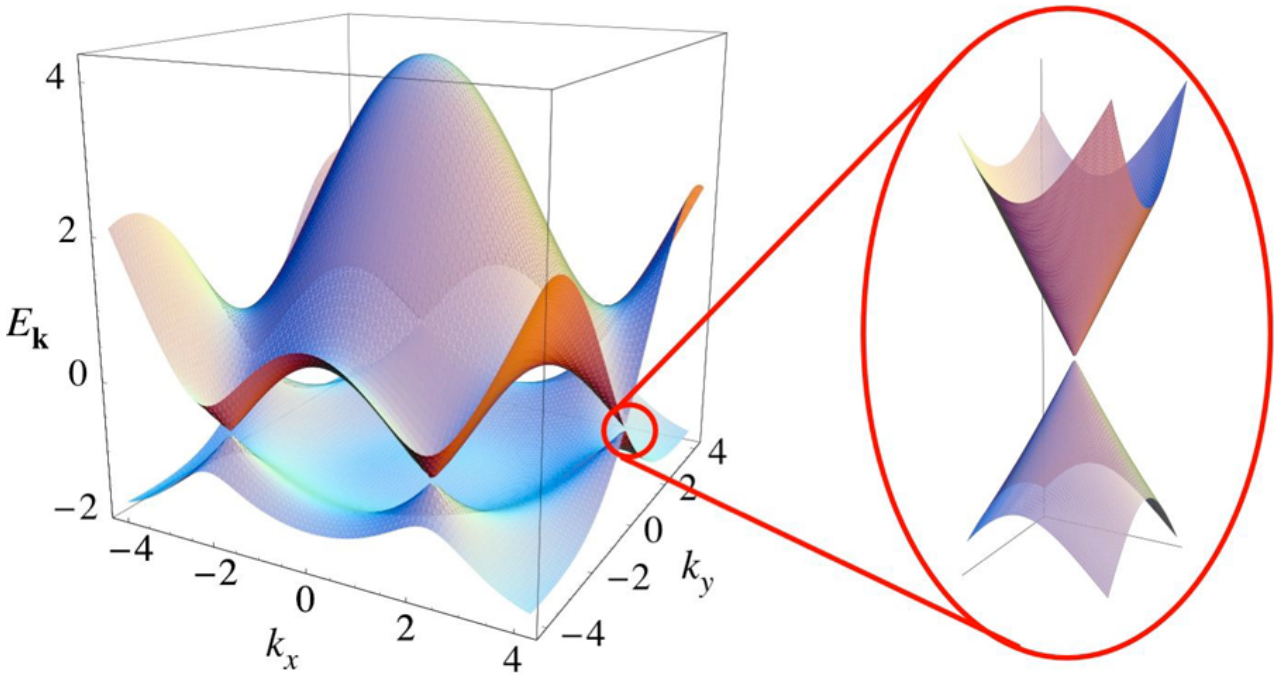


Examples of Dirac cones in electronic structure: Graphene



- 2D sheet of carbon
- 2D-Dirac cones (along k_x and k_y)
- up-down electrons are degenerate
- Fermi surface consists of just points.

Electronic structure of graphene:



http://faraday.fc.up.pt/cfp

Weyl equation

Dirac equation for massless spin-$\frac{1}{2}$ particles ($m_0 = 0$) $\rightarrow$ Weyl equation (in particle physics describing neutrino)

$$\begin{bmatrix} 0 & c\boldsymbol{\sigma}\cdot\mathbf{p} \\ c\boldsymbol{\sigma}\cdot\mathbf{p} & 0 \end{bmatrix} \begin{bmatrix} \varphi_L \\ \varphi_R \end{bmatrix} = |\mathbf{p}|c \begin{bmatrix} \varphi_L \\ \varphi_R \end{bmatrix}$$

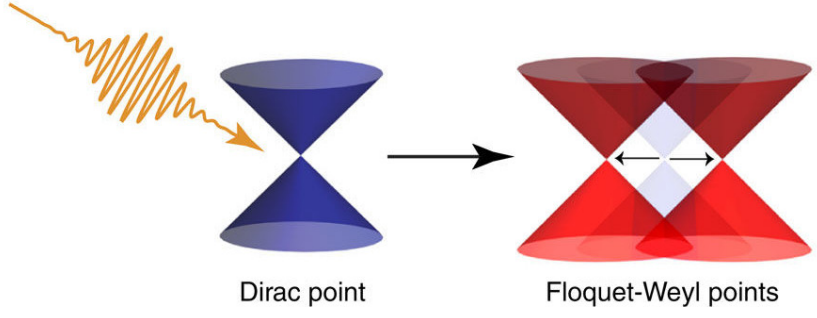
which can be rewritten to

$$[|\mathbf{p}| + \boldsymbol{\sigma}\cdot\mathbf{p}]\varphi_L(\mathbf{p}) = 0 \quad (1)$$

$$[|\mathbf{p}| - \boldsymbol{\sigma}\cdot\mathbf{p}]\varphi_R(\mathbf{p}) = 0 \quad (2)$$

solutions: spin helicity is fixed with the direction of motion.

In solids, terminology 'Dirac', 'Weyl' is used for degenerate, non-degenerate spin states on the cone, respectively



Two level degenerate system: Maxwell equation

Lossless Maxwell equations describing photon (boson with spin=1)

$$i\begin{bmatrix} 0 & \nabla\times \\ -\nabla\times & 0 \end{bmatrix}\begin{bmatrix} \mathbf{E} \\ \mathbf{B} \end{bmatrix} = \omega \begin{bmatrix} \epsilon & \chi \\ \chi^\dagger & \mu \end{bmatrix}\begin{bmatrix} \mathbf{E} \\ \mathbf{B} \end{bmatrix}$$

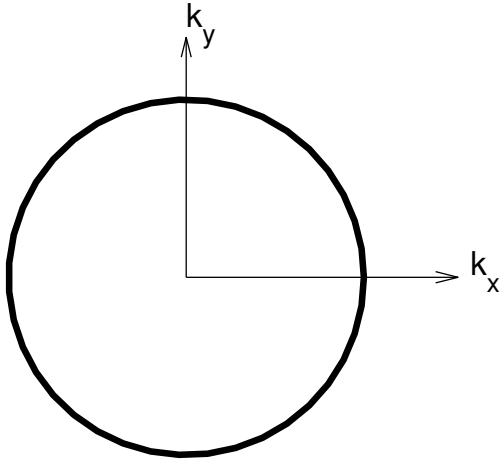
The main difference between fermions and bosons is time symmetry (fermions: $T^2 = -1$, bosons $T^2 = 1$, T is time operator)

Transport properties

Visualization of non-equilibrum electron states

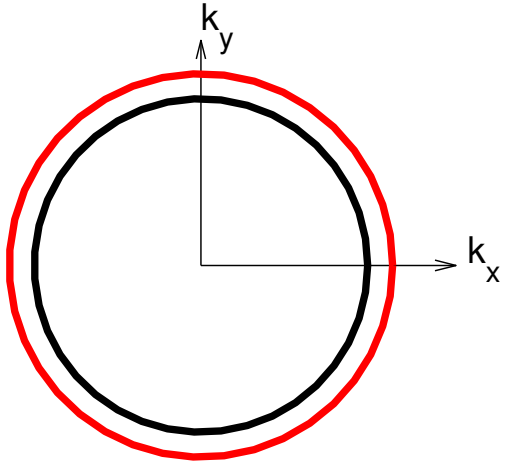
Sketch of equilibrum electron distribution (i.e. Fermi surface) and examples of non-equilibrum electron distributions

Equilibrun state:



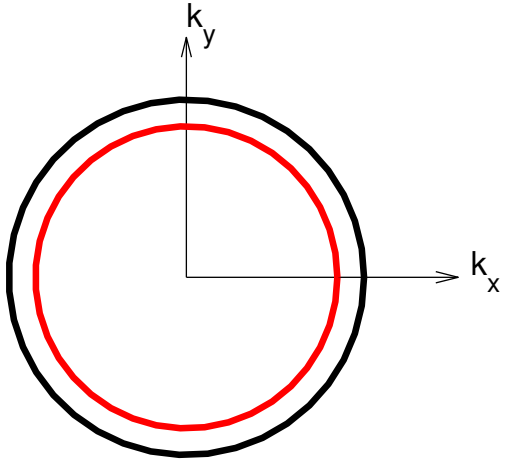
Electron accumulation:

$\Delta\mu > 0$



Electron accumulation:

$\Delta\mu < 0$



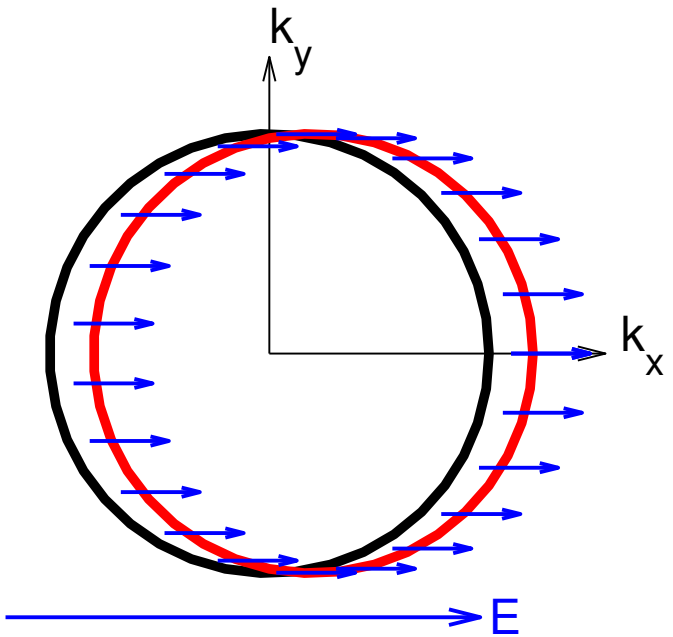
Introduction to electric conductivity

- applied electric field **E**
- all **k**-vectors move in the reciprocal space by $\mathbf{k} = \mathbf{k}_0 - \frac{e\mathbf{E}t}{\hbar}$
- it corresponds to speed of electrons

$$\mathbf{v} \approx \frac{\hbar}{m}(\mathbf{k} - \mathbf{k_0}) = \frac{e\mathbf{E}}{m}t$$

  i.e. classical acceleration of electrons by electric field

- this electron acceleration continues until electrons get scattered
- note: only electrons from unfilled bands contribute to the charge transfer
- finally, charge current is generated $\mathbf{j} = e\int_{\mathrm{BZ}} \mathbf{v}$



Electron dynamics in electric field

Electric field $\mathbf{E}$ is an perturbation to the Hamiltonian

$$\Delta H = e\phi(\mathbf{r}) = -e\mathbf{E}\cdot\mathbf{r}; \qquad \mathbf{E} = -\nabla\phi$$

ϕ being electrostatic potential.

- However, this perturbation breaks translational symmetry of the crystal $\Rightarrow$ Bloch theorem can not be applied.
- To introduce $\mathbf{E}$ without breaking time symmetry, $\mathbf{E}$ can be introduced by time-varying vector potential $\mathbf{A}(t)$,

$$\mathbf{E} = -\nabla\phi - \frac{\partial}{\partial t}\mathbf{A}$$

$$\mathbf{A}(t) = -\mathbf{E}t$$

Electron dynamics in electric field

Then, time dependent Hamiltonian has form

$$H(t) = \frac{1}{2m}[\mathbf{p} + e\mathbf{A}(t)]^2 + V(\mathbf{R})$$
$$= \frac{1}{2m}[\hbar\mathbf{q}]^2 + V(\mathbf{R})$$

- $\hbar\mathbf{q} = \hbar(\mathbf{k} + e\mathbf{A}(t))$ is (time independent) canonical monentum

$\Rightarrow$ $\mathbf{q}$ is still a good quantum number, with $\dot{\mathbf{q}} = 0$

- $\mathbf{p} = \hbar\mathbf{k} = \hbar(\mathbf{q} - \mathbf{A}(t))$ is momentum.

$\Rightarrow$ change of momentum $\mathbf{k}$ is simply

$$\dot{\mathbf{k}} = -\frac{e}{\hbar}\mathbf{E}$$

Electron dynamics in electric field

Substituting $\dot{\mathbf{k}} = -\frac{e}{\hbar}\mathbf{E}$ to transport equation

$$\dot{\mathbf{k}} = -\frac{e}{\hbar}\left(\mathbf{E} + \dot{\mathbf{r}} \times \mathbf{B}\right)$$
$$\dot{\mathbf{r}} = \frac{1}{\hbar}\frac{\partial \epsilon_n(\mathbf{k})}{\partial \mathbf{k}} - \dot{\mathbf{k}} \times \mathbf{\Omega}_n(\mathbf{k})$$

We got speed of Bloch electron in the crystal (in absence of scattering)

$$\mathbf{v}_n(\mathbf{k}) = \frac{e\mathbf{E}}{m}t - \frac{e}{\hbar}\mathbf{E} \times \mathbf{\Omega}_n(\mathbf{k})$$

→ the first term describes conductivity of the electronds (completly filled bands to not contribute to the conductivity).

→ the second term describes anomalous conductivity, i.e. $\mathbf{v} \perp \mathbf{E}$

(Ordinary) electric conductivity

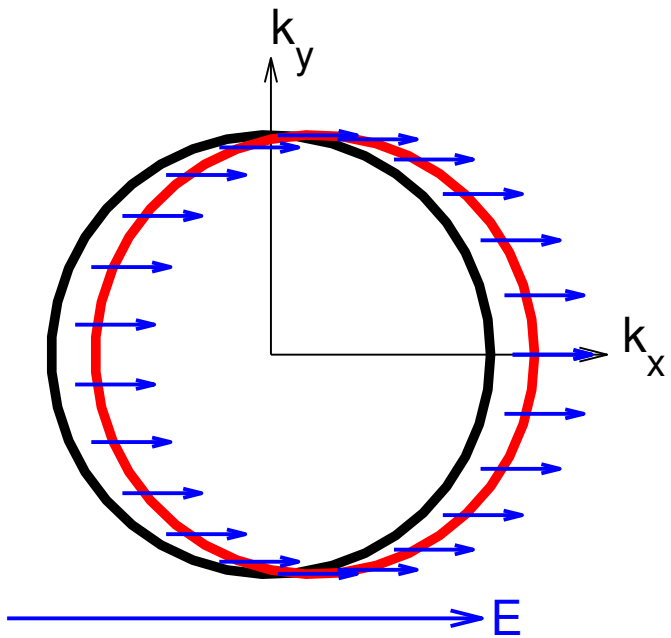
the speed of electron in solids (the first term):

$$\dot{\mathbf{r}} = \frac{1}{\hbar}\frac{\partial \epsilon_n(\mathbf{k})}{\partial \mathbf{k}}$$

can be approximately expressed as (assuming parabolic dispersion $\epsilon \sim (\mathbf{k}-\mathbf{k}_0)^2$):

$$\begin{aligned}\mathbf{v} \approx & \frac{1}{\hbar}\frac{\partial}{\partial \mathbf{k}}\epsilon(\mathbf{k}) = \\ = & \frac{1}{\hbar}\frac{\partial}{\partial \mathbf{k}}\left[\frac{\hbar^2}{2m}(\mathbf{k}-\mathbf{k}_0)^2\right] \\ = & \frac{\hbar}{m}(\mathbf{k}-\mathbf{k}_0) = \frac{\hbar}{m}\dot{\mathbf{k}}t = \frac{e\mathbf{E}}{m}t\end{aligned}$$

providing just simple acceleration of the electron by electric field



Anomalous electric conductivity

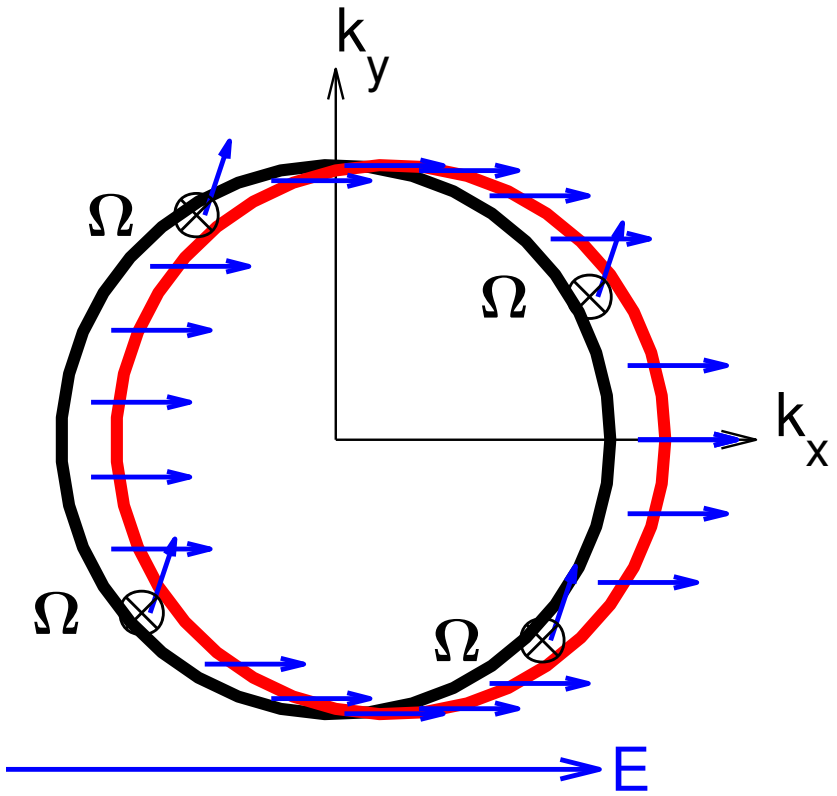
we add non-zero Berry curvature $\mathbf{\Omega}$ to our sketch of electron states

- Berry curvature on Fermi surafce is a point/line feature.
- here, we assume crystal with:
  - → time symmetry is broken
  - → inversion symmetry is present

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

⇒ due to equal direction of $\mathbf{\Omega}$, all anomalously scattered electrons are scattered in one direction (up), $\mathbf{v} \sim \mathbf{E} \times \mathbf{\Omega}$

⇒ anomalous (Hall) current, $\mathbf{j}_{\mathrm{Hall}} \perp \mathbf{E}$ is created, due to break of time symmetry



Anomalous electric conductivity

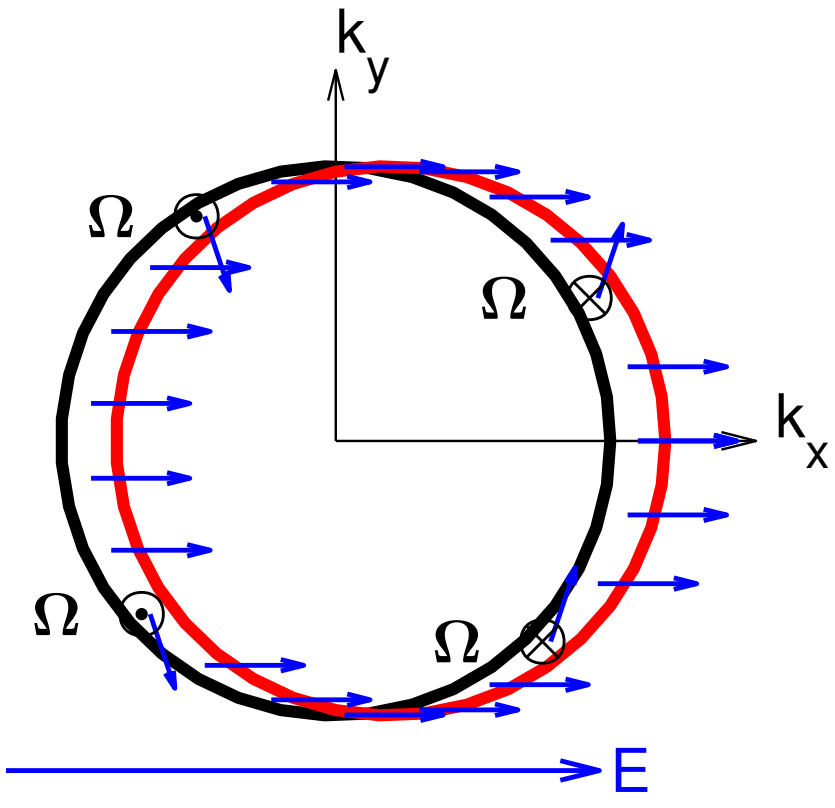
now, add non-zero Berry curvature, but with broken inversion symmetry

- here, we assume crystal with:
  - → inversion symmetry is broken
  - → time symmetry is present

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

⇒ due to different direction of $\mathbf{\Omega}$, there is no net current perpendicular to $\mathbf{E}$

⇒ anomalous (Hall current), $\mathbf{j}_{\mathrm{Hall}} \perp \mathbf{E}$ is NOT created, due to presence of time symmetry



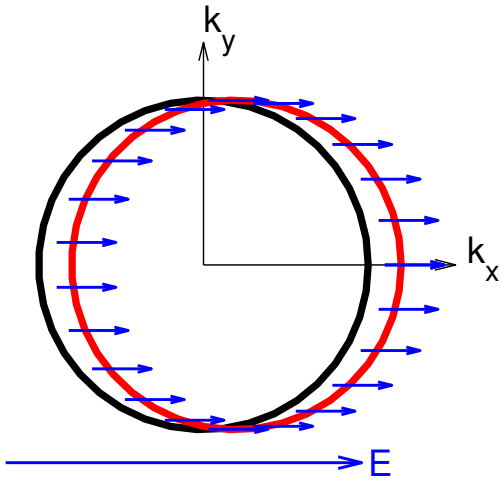
Visualization of non-equilibrum electron states

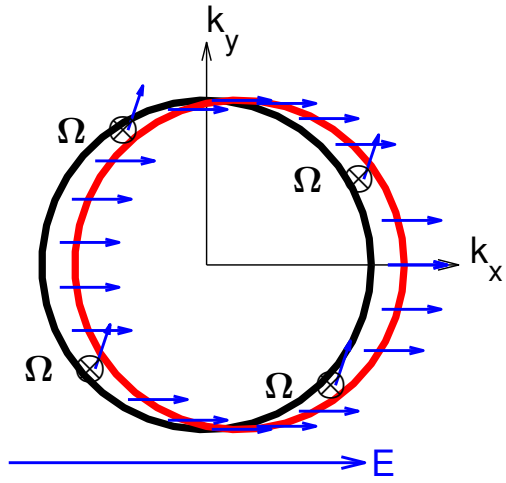
Applied electric field **E** in x-direction
$\Rightarrow$ charge current is generated

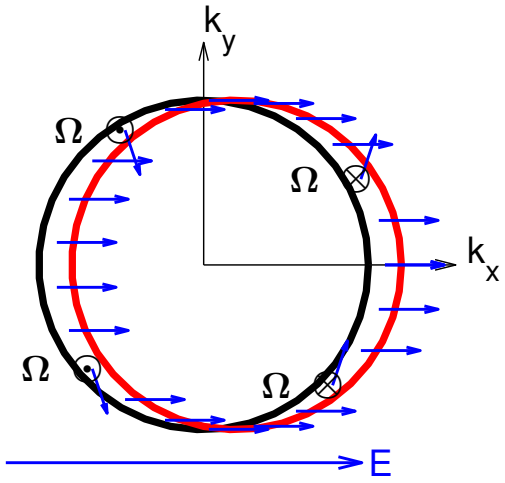
No Berry curvature

Berry curvature
no time symmetry
inversion symmetry
$\Omega(\mathbf{k}) = \Omega(-\mathbf{k})$

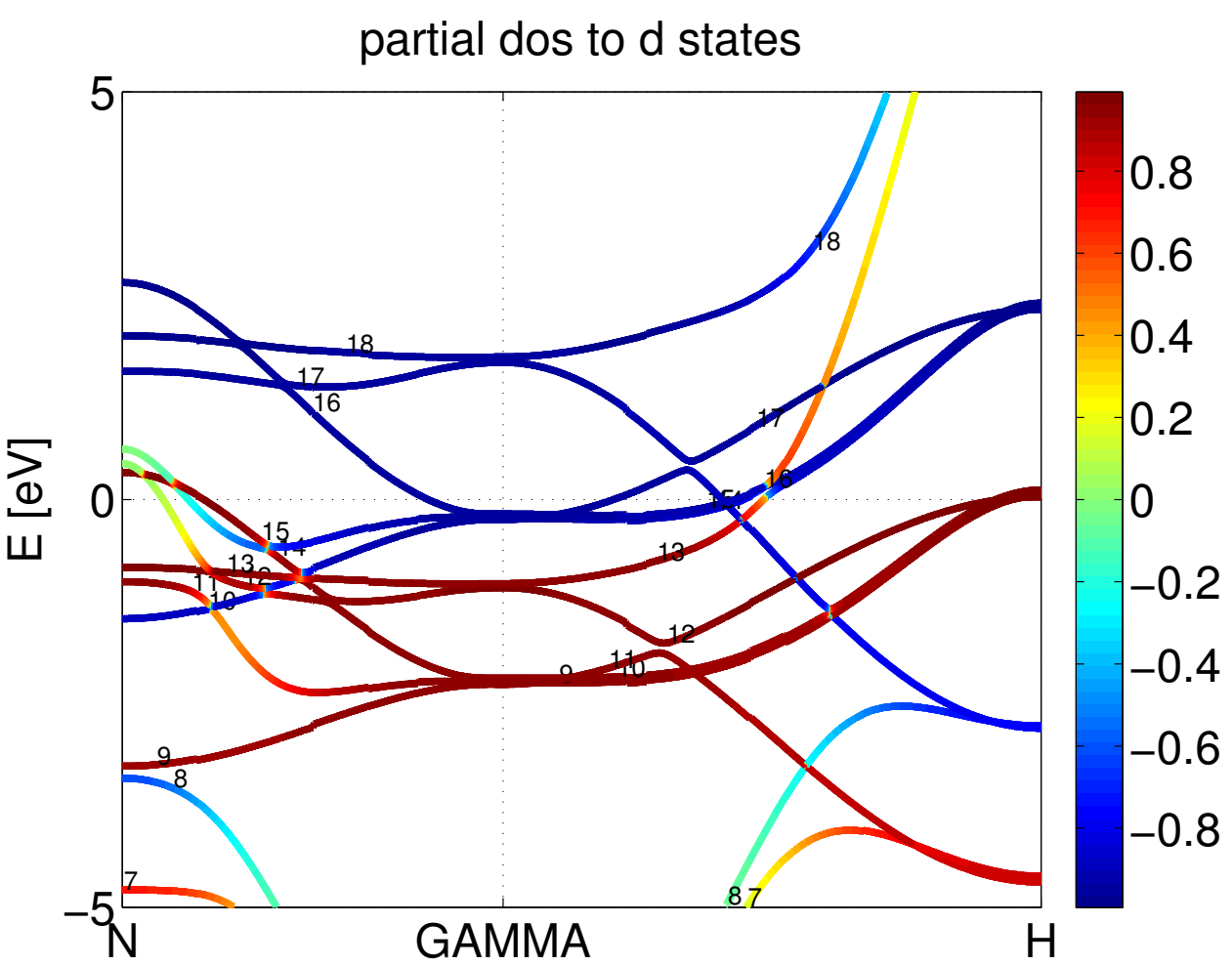
Berry curvature
no inversion symmetry
time symmetry
$\Omega(\mathbf{k}) = -\Omega(-\mathbf{k})$



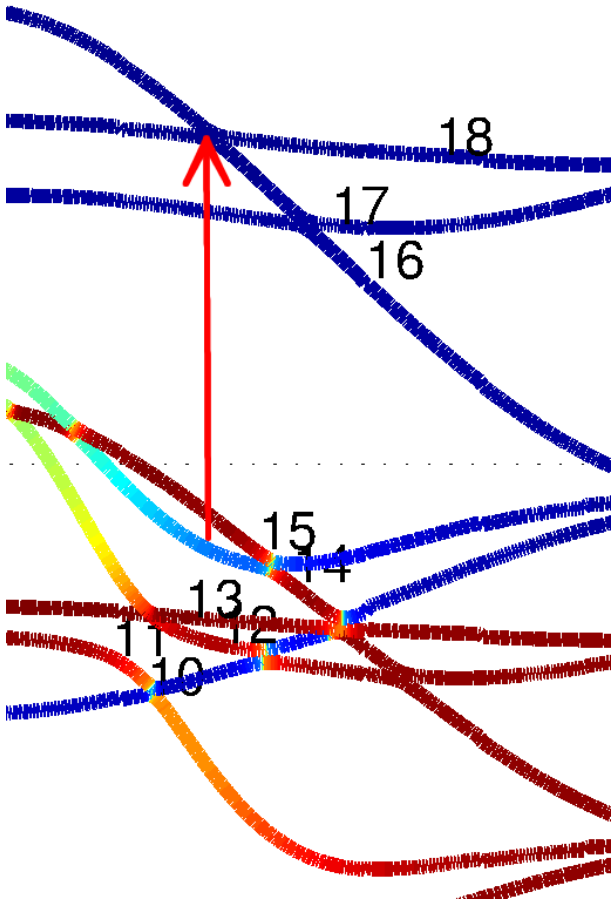


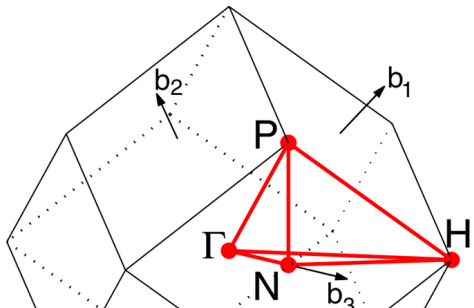


Examples of Berry curvatures on bcc Fe

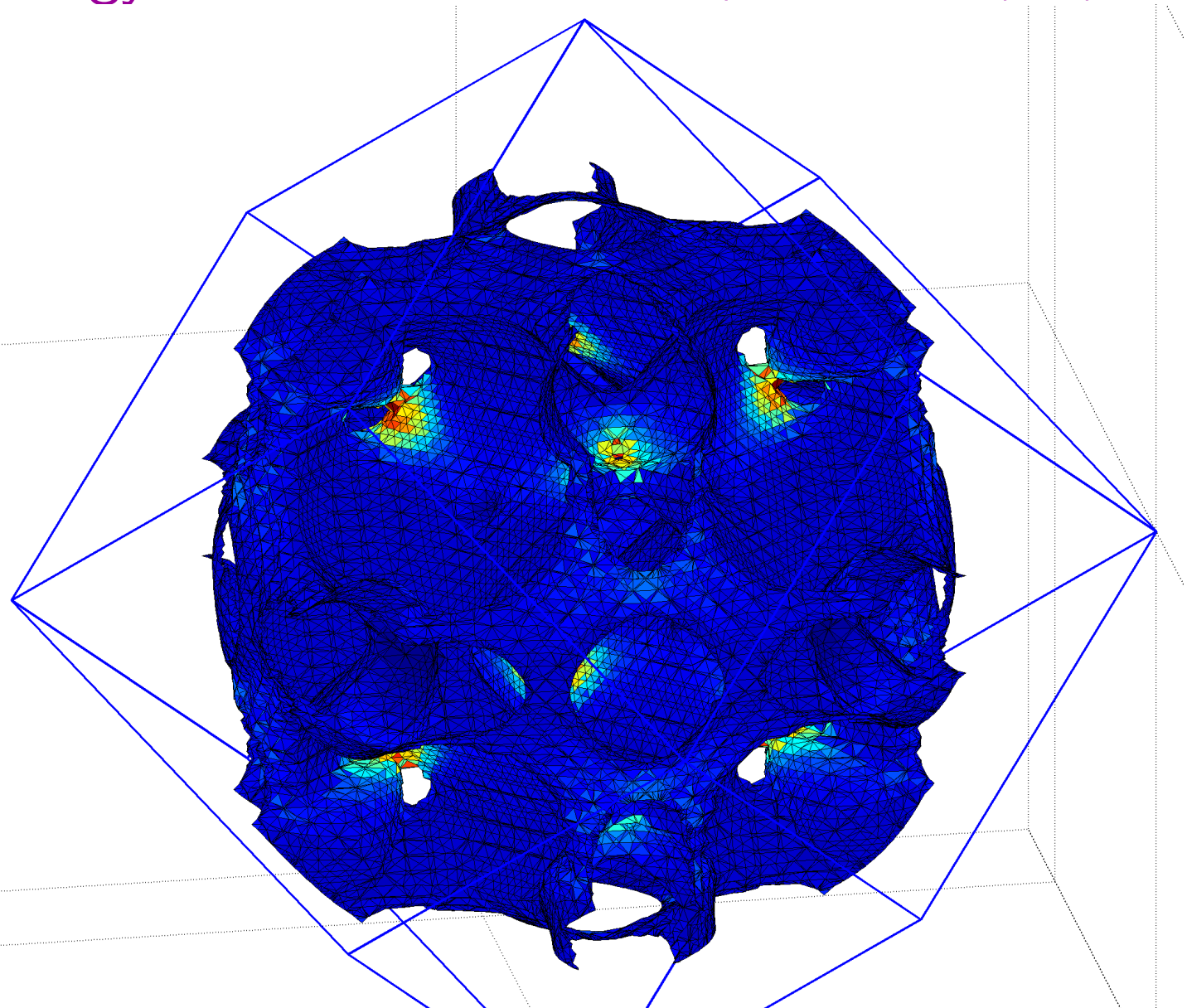


Color: projection to d-states:

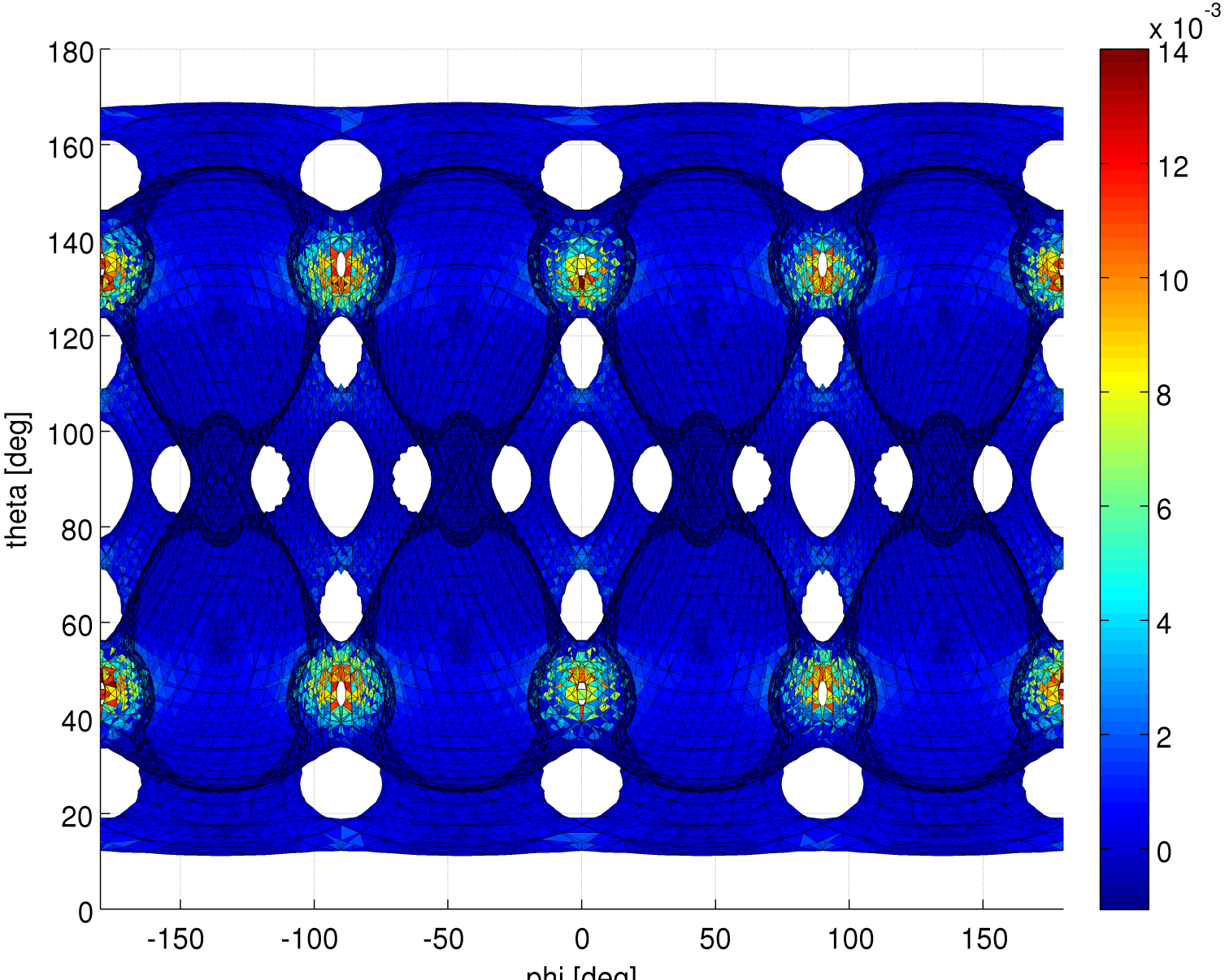




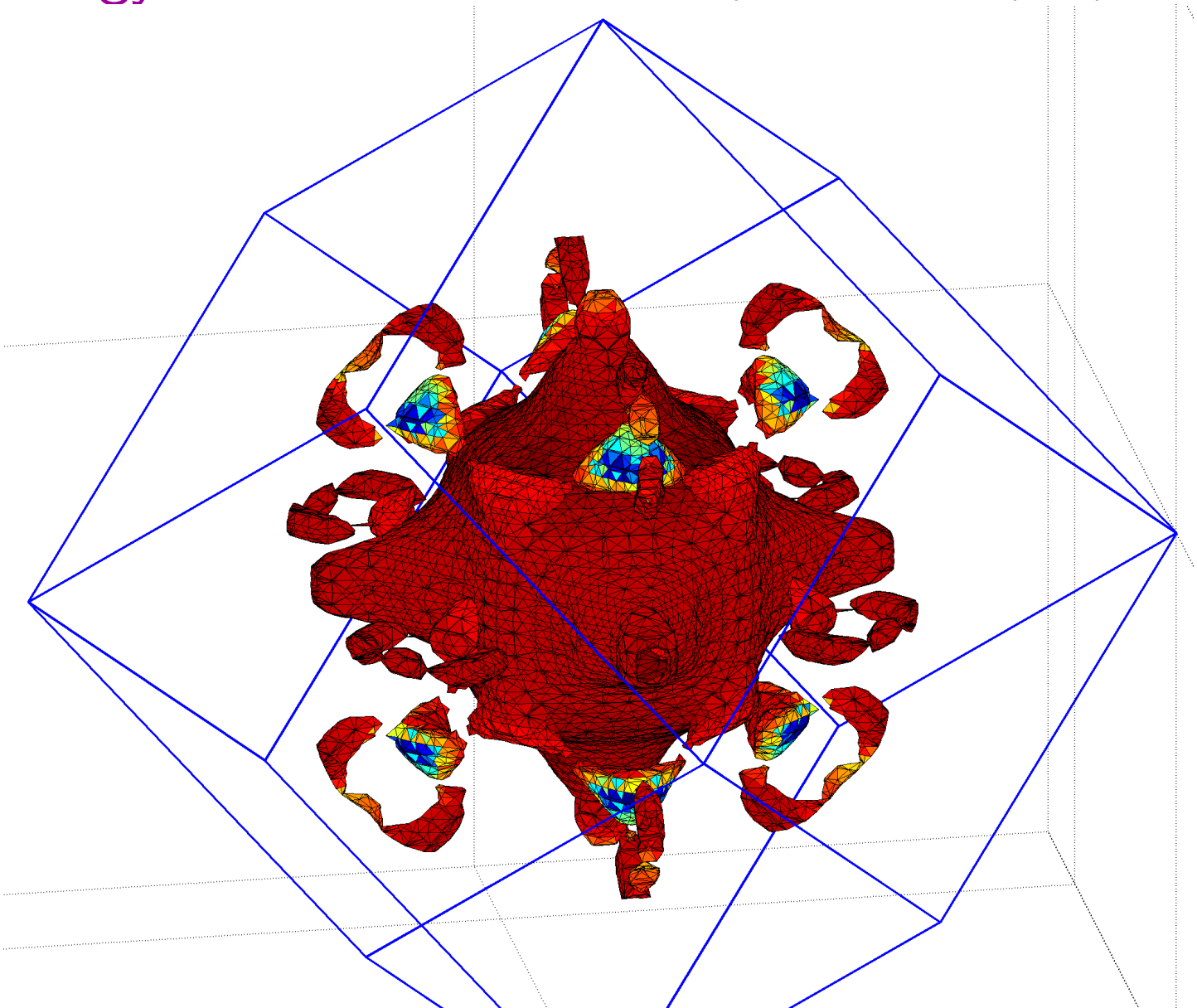
isoenergy surface $E = 2.23\,eV$, bands 14,17, color=Ω_z



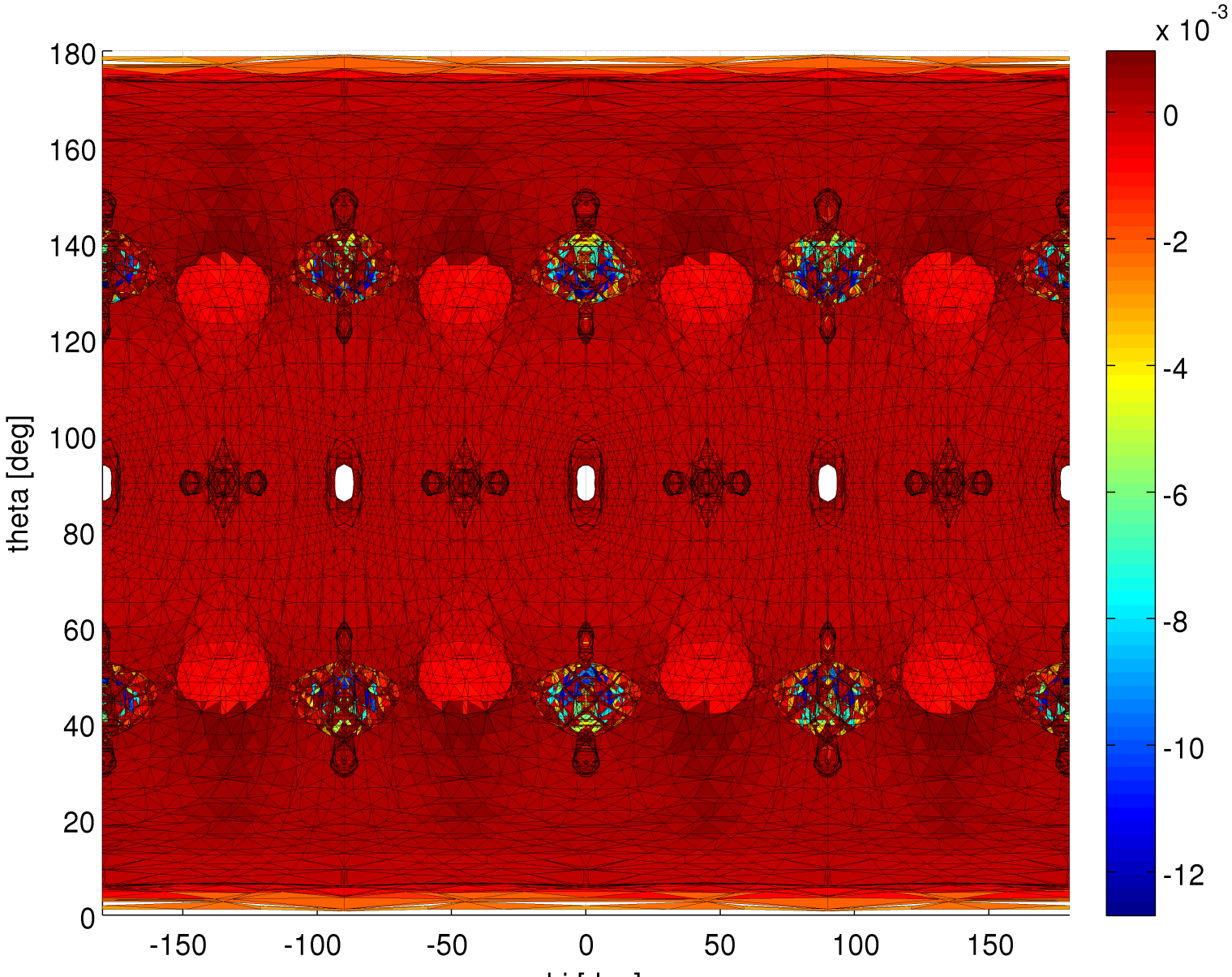
isoenergy surface $E = 2.23\,eV$, bands 14, 17, 2D view



isoenergy surface $E = 2.35\,eV$, bands 14,18, color=Ω_z

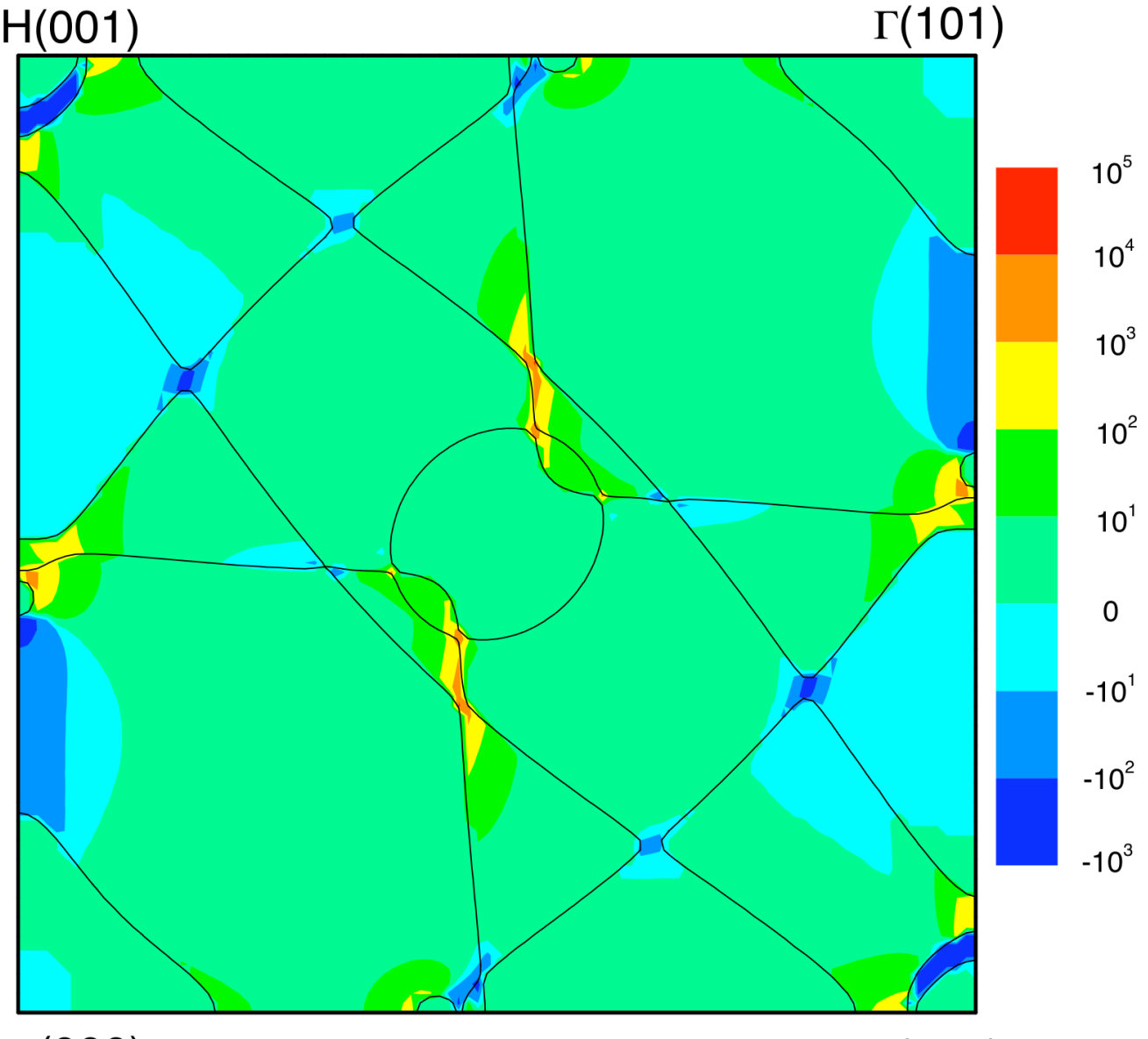


isoenergy surface $E = 2.35\,eV$, bands 14, 18, 2D view



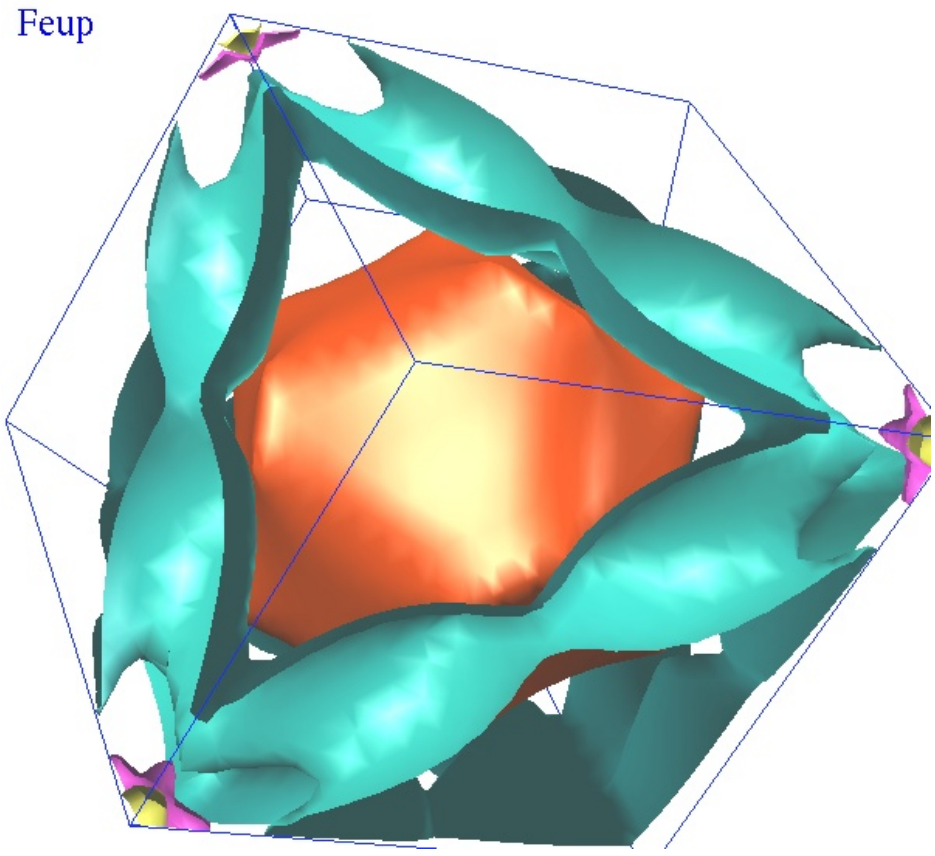
Integrated Berry curvature on bcc Fe

Fermi surface in (010) plane (solid lines) and the integrated Berry curvature $-\Omega_z(\mathbf{k})$ in atomic units (color map) of fcc Fe. From Yao et al.,PRL, 2004.

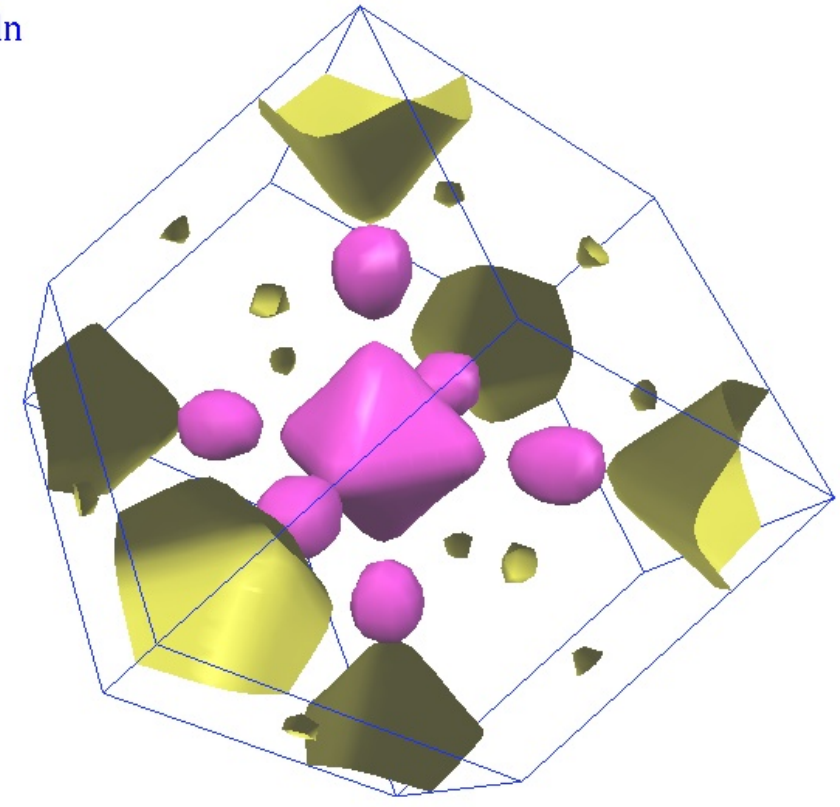


Fermi surface on bcc Fe

Fermi surface for up-spins:



Fermi surface for down-spins:



Relation between Berry curvature and Kubo formula

Berry curvature: dc Hall conductivity

Conductivity in x-direction, when field is applied in y-direction:

$$
\begin{aligned}
j_x &= -ev_x \\
&= -e\sum_n \int_{BZ} \frac{d^3\mathbf{k}}{(2\pi)^3} f_n(\mathbf{k}) v_x \\
&= -\frac{e^2}{\hbar}\sum_n \int_{BZ} \frac{d^3\mathbf{k}}{(2\pi)^3} f_n(\mathbf{k}) \left(\mathbf{E}\times\boldsymbol{\Omega}_n(\mathbf{k})\right)_x \\
&= -\frac{e^2}{\hbar}\sum_n \int_{BZ} \frac{d^3\mathbf{k}}{(2\pi)^3} f_n(\mathbf{k}) E_y \Omega_{n,z}(\mathbf{k})
\end{aligned}
$$

where $f_n(\mathbf{k})$ is Fermi distribution function.
Note, amplitude (j_x) is perpendicular to applied force (E_x).

Berry curvature: dc Hall conductivity

off-diagonal (Hall conductivity) given by Berry curvature writes:

$$\sigma_{xy} = \frac{j_x}{E_y} = -\frac{e^2}{\hbar} \sum_n \int_{BZ} \frac{d^3\mathbf{k}}{(2\pi)^3} f_n(\mathbf{k}) \Omega_{n,z}(\mathbf{k})$$

On the other hand, the well-know relation describing conductivity (and light absorption) is Kubo formula:

$$\sigma_{xy} = i\frac{e^2}{m_e^2\hbar} \sum_n \sum_{n' \neq n} \int_{BZ} \frac{d^3\mathbf{k}}{(2\pi)^3} \left[f_n(\mathbf{k}) - f_{n'}(\mathbf{k})\right] \times \frac{\langle n|p_x|n'\rangle \langle n'|p_y|n\rangle - \langle n|p_y|n'\rangle \langle n'|p_x|n\rangle}{(\epsilon_n - \epsilon_{n'})^2}$$

How to relate both expressions?

Relation between Berry curvature and Kubo formula II

First, let us establish identity:

$$\begin{aligned}\epsilon_{n'} \langle \nabla_{\mathbf{k}} n | n' \rangle &= \langle \nabla_{\mathbf{k}} n | H n' \rangle \\ &= \langle n | \nabla_{\mathbf{k}} H | n' \rangle + \langle n | H | \nabla_{\mathbf{k}} n' \rangle \\ &= \langle n | \nabla_{\mathbf{k}} H | n' \rangle + \epsilon_n \langle n | \nabla_{\mathbf{k}} n' \rangle\end{aligned}$$

taking into account $\langle n | \nabla_{\mathbf{k}} n' \rangle = \langle n | \nabla_{\mathbf{k}} n' \rangle = \langle n | \nabla_{\mathbf{k}} | n' \rangle$ we obtain

$$\langle \nabla_{\mathbf{k}} n | n' \rangle (\epsilon_{n'} - \epsilon_n) = \langle n | \nabla_{\mathbf{k}} H | n' \rangle$$

Relation between Berry curvature and Kubo formula II

- applying the identity using complete set of orthonormal basis vectors $\mathbf{1} = \sum_m |m\rangle \langle m|$

$$\mathbf{\Omega} = \nabla_{\mathbf{k}} \times i \langle n|\nabla_{\mathbf{k}} n\rangle = i \langle \nabla_{\mathbf{k}} n| \times |\nabla_{\mathbf{k}} n\rangle = i \sum_{m \neq n} \langle \nabla_{\mathbf{k}} n|m\rangle \times \langle m|\nabla_{\mathbf{k}} n\rangle$$

- substituting $\langle \nabla_{\mathbf{k}} n|m\rangle (\epsilon_m - \epsilon_n) = \langle n|\nabla_{\mathbf{k}} H|m\rangle$

$$\mathbf{\Omega}_n = i \sum_{n \neq m} \frac{\langle n|\nabla_{\mathbf{k}} H|m\rangle \times \langle m|\nabla_{\mathbf{k}} H|n\rangle}{(\epsilon_n - \epsilon_{n'})^2}$$

Relation between Berry curvature and Kubo formula II

- Taking into account

$$\nabla_{\mathbf{k}} H = \frac{\hbar^2}{m}\mathbf{k} = \frac{\hbar}{m}\mathbf{p}$$

Berry curvature can be expressed by matrix elements of momentum:

$$\mathbf{\Omega}_n = i\frac{\hbar^2}{m_e}\sum_{n\neq m}\frac{\langle n|\mathbf{p}|m\rangle \times \langle m|\mathbf{p}|n\rangle}{(\epsilon_n - \epsilon_m)^2}$$

$\rightarrow$ this form of Berry curvature corresponds to Kubo formula

$\rightarrow$ this form is used to express Kubo formula by calculations (both analytical and numerical), to avoid gradient of wavefunctions.

Time reversal symmetry

Time reversal symmetry I

(according F. Haake, Time Reversal and Unitary Symmetries in Quantum Signatures of Chaos)

A classical Hamiltonian system is called time invariant, when for time reversal $t \to -t$, the solutions transforms as (conventional invariance):

$$t \to -t \qquad \mathbf{x} \to \mathbf{x} \qquad \mathbf{p} \to -\mathbf{p} \qquad \mathbf{L} \to -\mathbf{L} \qquad \mathbf{S} \to -\mathbf{S}$$
$$\psi \to T\psi$$

where T is time-reversal operator, being so-called antiunitary, defined as:

$$\langle T\psi | T\phi \rangle = \langle \psi | \phi \rangle^{\star} = \langle \phi | \psi \rangle$$

because

- overlap of two wavefunctions must be preserved
- explicit 'i' in Schrodinger equation; $i\hbar\partial\psi/\partial t = H\psi$

Time reversal symmetry II

Time reveral operator T is antiunitary $\Rightarrow$ T^2 is unitary, $|T^2| = 1$
$\Rightarrow$ time-reversal operator can be written as

$$T = UK$$

where K is complex conjugation and U is unitary operator
$\Rightarrow$ $T^2 = \pm 1$

- $T^2 = 1$ for spinless or spin-integer particles (e.g. photons)
- $T^2 = -1$ for spin-1/2 particles (electrons)

Note:

- Hamiltonian is non-dissipative (i.e. conserving phase-space volume according to Liouville theorem)

$\Rightarrow$ following discussions regarding time reversal does not work for dissipative system.

Note: unitary operator: $U^\star = U^{-1}$, i.e. complex conjugation equals inverse (e.g. U is rotation operator, keeping angles and lengths).

F. Haake, Time reveral and Unitary Symmetries, *Quantum signatures of chaos*, Springer

Spinless particle

Schrodinger equation $i\hbar\frac{\partial}{\partial t}\psi(\mathbf{x},t) = H\psi(\mathbf{x},t)$

Hamiltonian $H = \frac{\mathbf{p}^2}{2m} + V(x)$ is called time-reversal invariant when having solution $\psi(\mathbf{x},t)$ for t, there is another solution $\psi'(\mathbf{x},t')$ for $t' = -t$ uniquely related to $\psi(\mathbf{x},t)$.
In case of so-called conventional time reversal

$$t \to -t \qquad \mathbf{x} \to \mathbf{x} \qquad \mathbf{p} \to -\mathbf{p}$$
$$\psi(\mathbf{x}) \to \psi^\star(\mathbf{x}) = K\psi(\mathbf{x})$$

with K being operator of complex conjugation, with $K^2 = 1$.
Hence, in case of spinless particle, time reversal operator T equals operator of complex conjugation K, $T = K$

$$T\,|\psi\rangle = K\,|\psi\rangle = |\psi\rangle^\star$$

Spin-1/2 particle

Spin-1/2 particle requires reversal of spin under time reversal

$$\langle T\phi|\, T\mathbf{S}\psi\rangle = \langle T\phi|\, T\mathbf{S}\,T^{-1}|\, T\psi\rangle = -\langle\phi|\mathbf{S}|\psi\rangle$$

providing

$$T\mathbf{S}\,T^{-1} = -\mathbf{S}$$

$\Rightarrow$ operator T can not be solely complex conjugation
$\Rightarrow$ $T = UK$,

Spin-1/2 particle: derivation of form of T-operator

Derivation of $T = UK$ for spin-1/2 particle ($\mathbf{S} = \frac{\hbar}{2}\boldsymbol{\sigma}$):

$$T\sigma_i T^{-1} = -\sigma_i$$

U must have general form as (general form of any Hermitian 2x2 matrix)

$$U = \alpha\sigma_x + \beta\sigma_y + \gamma\sigma_z + \delta$$

we get only non-zero term $\beta = i$ and hence time operator for spin-1/2 particles is

$$T = i\sigma_y K = i \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} K = \exp[i\pi\sigma_y/2]K$$

Kramers' degeneracy

For any Hamiltonian invariant under time reversal

$$[H, T] = 0$$

its eigenvectors $|\psi_n\rangle$ and $|T\psi_n\rangle$ has equal eigenvalues E_n.

- for $T^2 = 1$: we can choose eigenvectors to follow $|\psi\rangle = |T\psi\rangle$ using combination $|\psi\rangle = a|\psi'\rangle + aT|\psi'\rangle$
- for $T^2 = -1$, $|\psi\rangle$ and $|T\psi\rangle$ are orthogonal

$$\langle\psi|T\psi\rangle = \langle T\psi|T^2\psi\rangle^\star = -\langle T\psi|\psi\rangle^\star = -\langle\psi|T\psi\rangle = 0$$

$\Rightarrow$ all eignevalues of H are double degenerate, with eigenvectors $|\psi\rangle$ and $T|\psi\rangle \equiv |T\psi\rangle$, called Kremers' degeneracy.
For example, in case of single-electron Hamiltonian without SOC and without B, spin-up and spin-down states are degenerates.

Kramers' degeneracy without geometric symmetries I

For $T^2 = -1$, we adopt basis

$$|1\rangle, \quad |T1\rangle, \quad |2\rangle, \quad |T2\rangle, \ldots |N\rangle, \quad |TN\rangle$$

General wavefunction can be written as

$$|\psi\rangle = \sum_m a_{mt+} |m\rangle + a_{mt-} |Tm\rangle$$
$$|T\psi\rangle = \sum_m a^\star_{mt+} |Tm\rangle - a^\star_{mt-} |m\rangle$$

As $|T\psi\rangle = UK|\psi\rangle$, U must have form

$$U_{mm} = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} = -i\sigma_y \qquad U_{mn} = 0 \text{ for } m \neq n$$

Kramers' degeneracy without geometric symmetries II

Similarly, Hamiltonian can be written as

$$h_{mn} = \begin{bmatrix} \langle m|H|n\rangle & \langle m|H|Tn\rangle \\ \langle Tm|H|n\rangle & \langle Tm|H|Tn\rangle \end{bmatrix}$$

where the matrix form of Hamiltonian element h_{mn} can be written using Pauli matrices and four real $h_{mn}^{(0...3)}$ with

$$h_{mn} = h_{mn}^{(0)}\mathbf{1} - i\mathbf{h}_{mn} \cdot \boldsymbol{\sigma}$$

This is similar form of Hamiltonian we discussed for two-level degenerate system
$\Rightarrow$ break of time symmetry when Hamiltonian contains terms not fulfilling time reversal symmetry (such as SOC) then in general off-diagonal terms are nonzero, diagonal terms do not equal
$\Rightarrow$ break of time symmetry provides splitting of eigenvalues and non-zero Berry curvature.

Kramers' degeneracy without geometric symmetries III

In case of photons, $T^2 = 1 \Rightarrow$ Hamiltonian element

$$h_{mn} = \begin{bmatrix} \langle m|H|n\rangle & \langle m|H|Tn\rangle \\ \langle Tm|H|n\rangle & \langle Tm|H|Tn\rangle \end{bmatrix}$$

is diagonal, $h_{mn} = h^{(0)}_{mn}\mathbf{1}$
$\Rightarrow$ break of time symmetry (i.e. Hamiltonian non-invariant under time reversal, $[H, T] \neq 0$) does not provide energy splitting or Berry curvature of photon wavefunction
$\Rightarrow$ splitting of photon eigenvalues can be obtained by interaction with solids (magnetooptics)

Spin-orbit interaction of light

Spin-orbit interaction of light

K.Y. Bliokh, Nature Photon. 9, 796 (2015)
Similar to spin-orbit coupling of electron, there is spin-orbit coupling also for photon (for light beam).

- Spin-orbit interaction of electron: connect spin wavefunction and space wavefunction
- Spin orbit coupling of photon: connects beam trajectory and its polarization state (also know as optical spin-Hall effect).

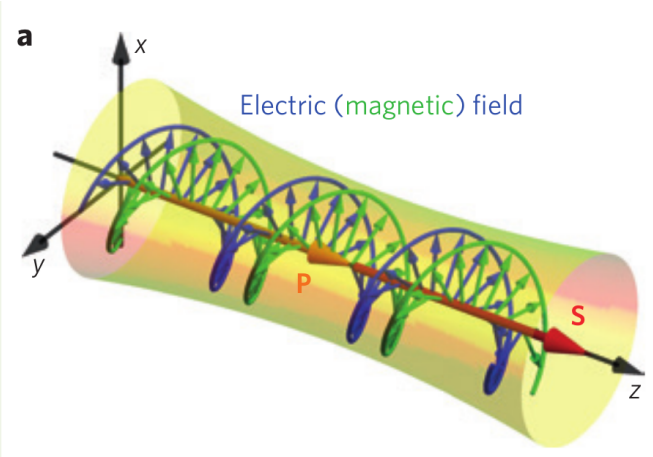
Angular momenta of light I

Spin angular momentum S:

degree of circular polarization (helicity)

$\sigma = (-1, 1)$

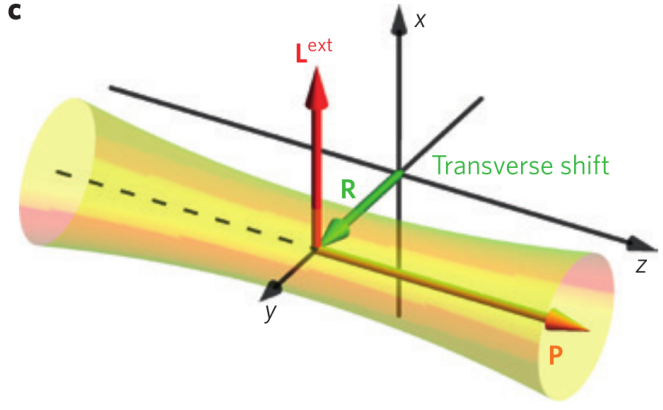
$\mathbf{S} = \sigma \frac{\mathbf{k}}{k} = \sigma \frac{\mathbf{p}}{p}$



Extrinsic orbital angular momentum $\mathbf{L}^{ext}$:

determined by the trajectory of the beam $\mathbf{R}$

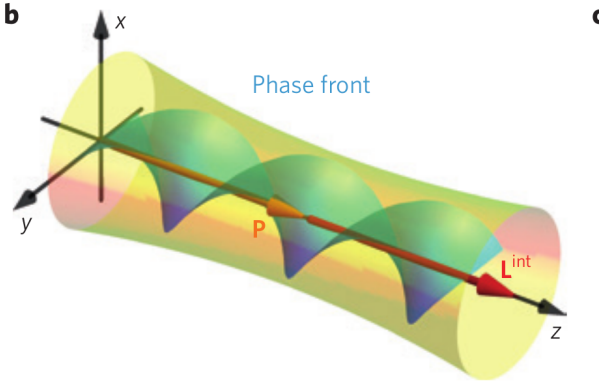
$\mathbf{L}^{ext} = \mathbf{R} \times \mathbf{p}$

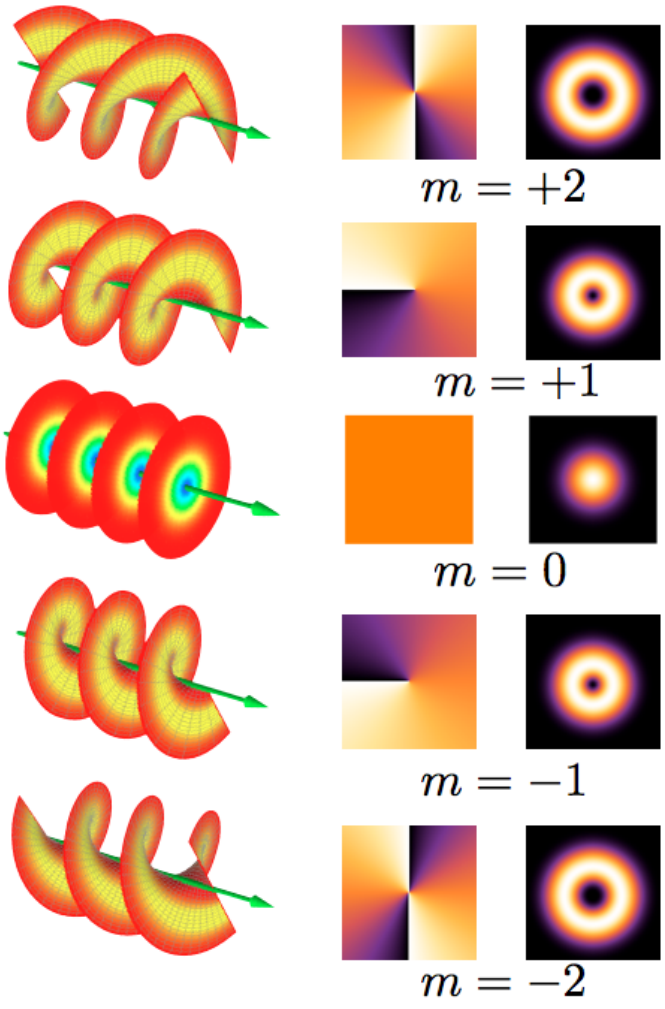


Angular momenta of light II

Intrinsic angular momentum L^{int}:
helical phase front: phase of the beam depends on position inside beam, approximately
$E(r, z, \phi) \approx E_0(r, z) \exp[il\phi]$, where r, z, ϕ are coordinates in cylindrical coordinates.

$$L^{int} = l\frac{\mathbf{k}}{k}, \qquad l \in \mathbb{Z}$$



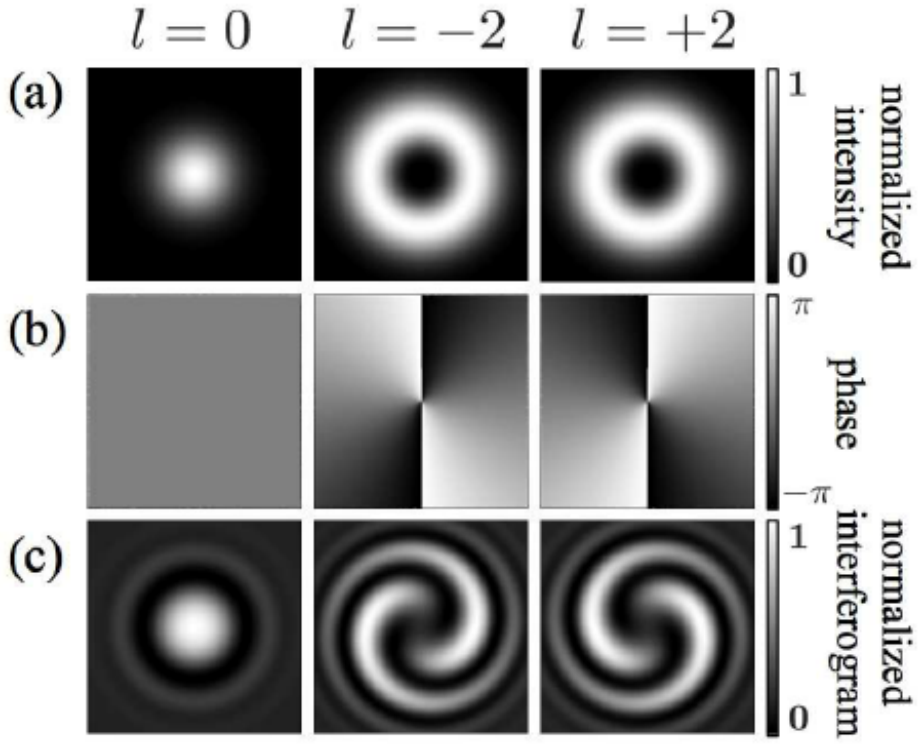


Angular momenta of light III

Intrinsic angular momentum L^{int}:

Laguerre-Gaussian modes:

- symmetrical beams with non-zero intrinsic angular momentum of light
- also called optical vortex with topological charge l



$$u(r, z, \phi) = \exp\left(-ik\frac{r^2}{2R(z)}\right)\exp(-il\phi)\,\exp(-ikz)\,\exp(i\psi(z))$$

Helical mode conversion using conical reflector, Optics Express **20**, 14064 (2012)

Optical spin Hall effect I

Interactions between those three angular momenta of light represents spin-orbit coupling of light.

Example: optical spin Hall effect:

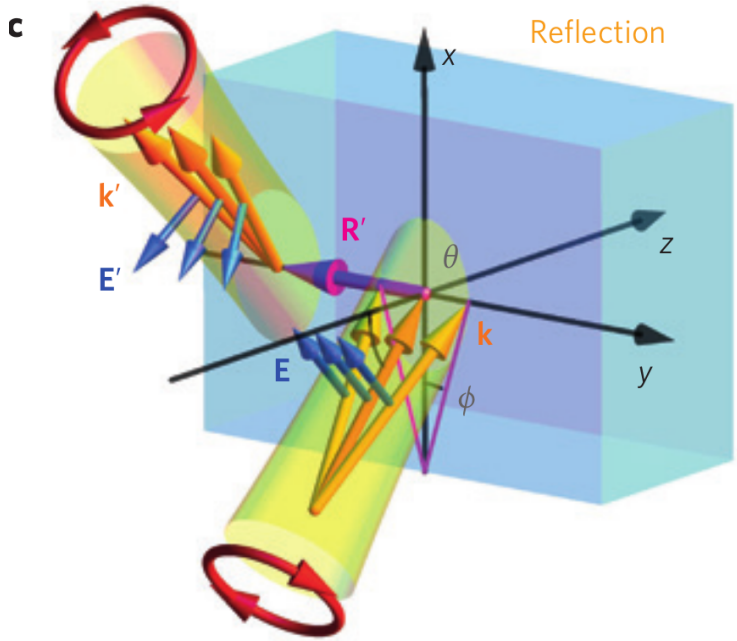
The light beam on reflection displaces (shifts) according to the beam helicity σ. Consequence of total angular momentum conservation:

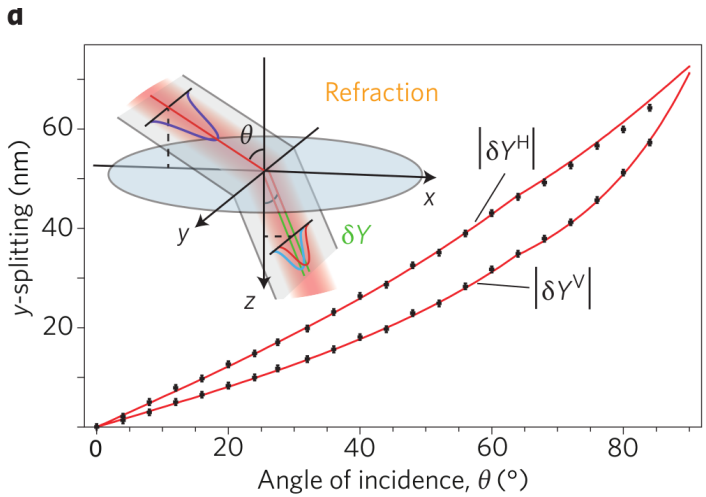
$$\mathbf{J} = \mathbf{S} + \mathbf{L}^{ext} = \mathbf{S} + \mathbf{R} \times \mathbf{p}$$

adjusting coordinates that incident beam has $\mathbf{R} = 0$ and hence $\mathbf{L}^{ext} = 0$

$$\mathbf{S} - \mathbf{S}' \approx \mathbf{R}' \times \mathbf{p}'$$

K.Y. Bliokh, Nature Photon. 9, 796 (2015)





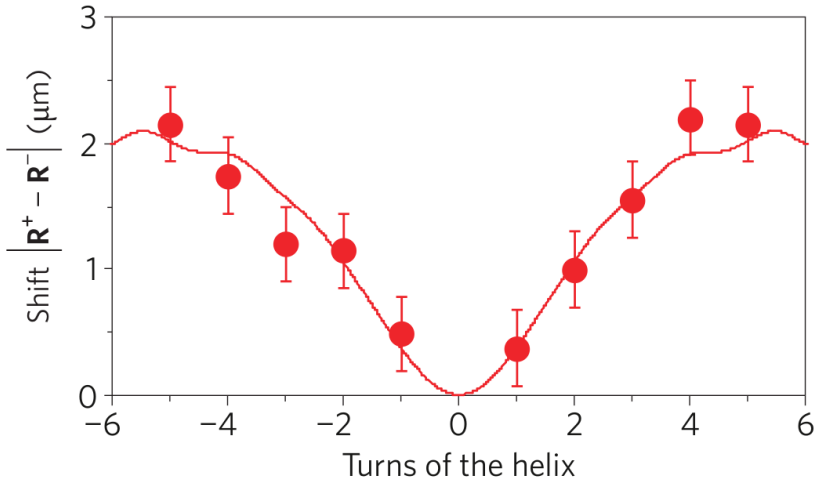
Optical spin Hall effect II

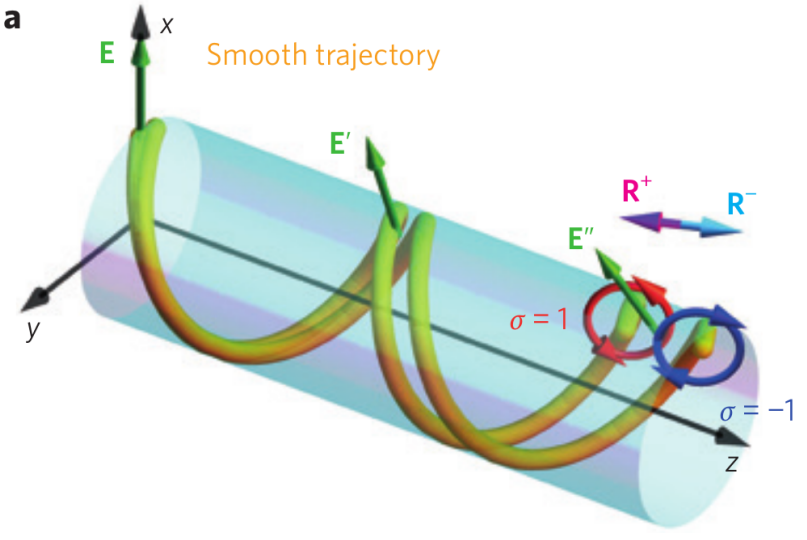
$\mathbf{J} = \mathbf{S} + \mathbf{L}^{ext} = \mathbf{const.}$
displacement of beam due to light helicity inside the glass cylinder with gradient of refraction index.

$$\dot{\mathbf{p}} = \nabla n(\mathbf{R}) \qquad \dot{\mathbf{R}} = \frac{\mathbf{p}}{p} - \frac{\sigma}{k_0}\frac{\mathbf{p}\times\dot{\mathbf{p}}}{p^3}$$

(overdot denotes derivation according to the trajectory, $\mathbf{p} = \mathbf{k}/k_0$ is dimensionless momentum)

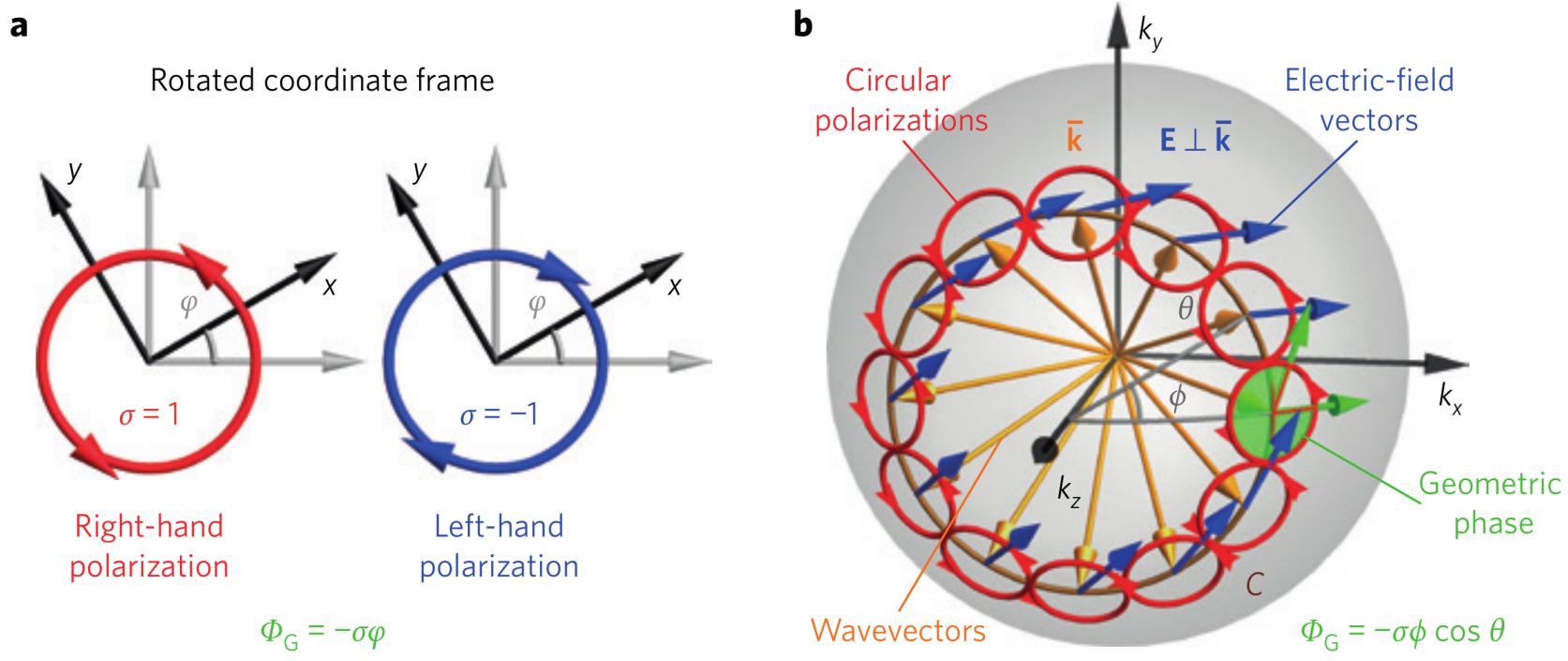
Bliokh Nature Photon. 2, 748 (2008)





Optical spin Hall effect III

The relation between light polarization and trajectory can be laso understand in terms of Berry phase:



Phase of the light wave varies as light propagetes inside glass cylinder providing cyclic variation of wavevector direction **p**

Optical spin Hall effect IV

Berry connection:

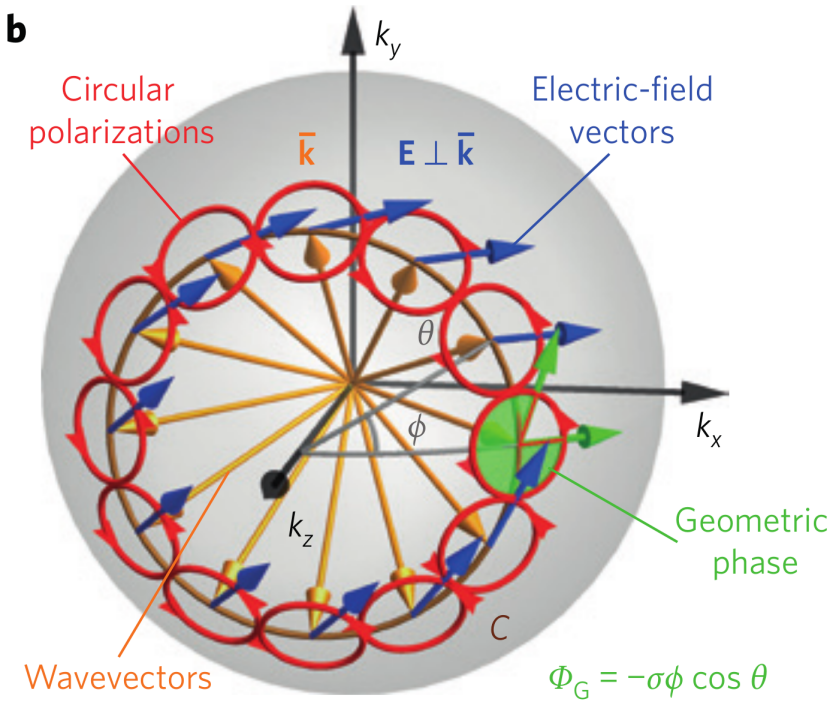
$$\mathbf{A} = -i\mathbf{E}^{\sigma} \cdot \nabla_{\mathbf{k}} \mathbf{E}^{\sigma}$$

Berry curvature:

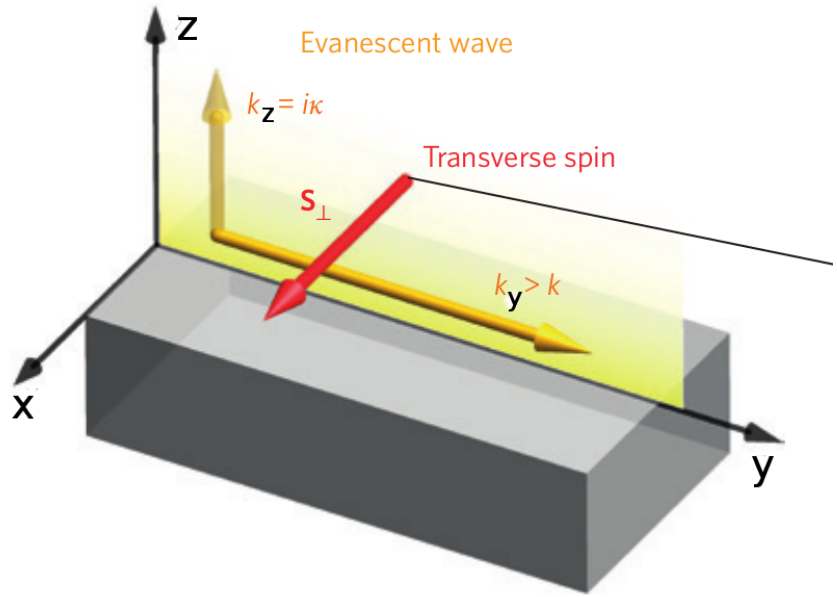
$$\mathbf{\Omega}^{\sigma}(\mathbf{k}, \sigma) = \nabla \times \mathbf{A} = \sigma \frac{\mathbf{k}}{k^3}$$

Geometric (Berry) phase:

$$\begin{aligned} \Phi_G &= \int_C \mathbf{A} \mathrm{d}\mathbf{k} = \int_S \Omega \mathrm{d}S_{\mathbf{k}} \\ &= 2\pi\sigma(1 - \cos\theta) \end{aligned}$$

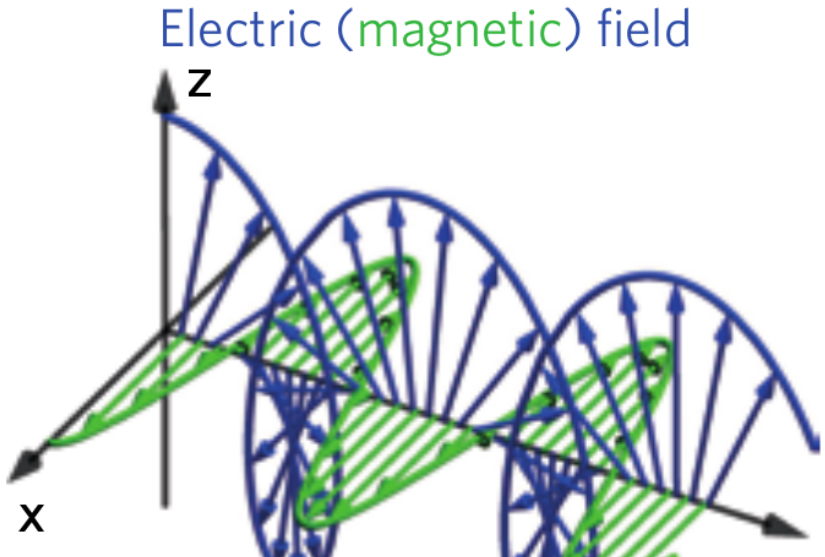


Spin transfer by evanescent wave

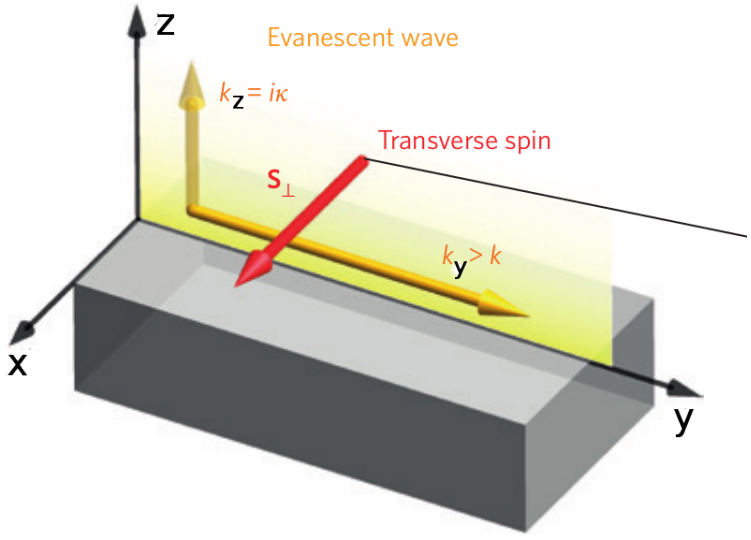


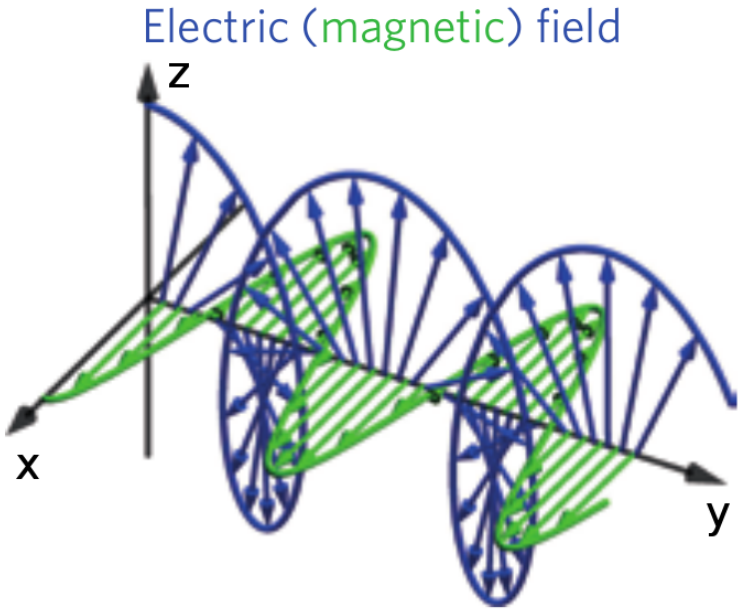
Electrical field of the evanescent wave (propagation along y, recall $\mathbf{E} \cdot \mathbf{k} = 0$):

$$\mathbf{k} = \begin{bmatrix} 0 \\ k_y \\ iK \end{bmatrix} \qquad \mathbf{E} = \begin{bmatrix} 0 \\ i(-K/k_y)E_z \\ E_z \end{bmatrix}$$

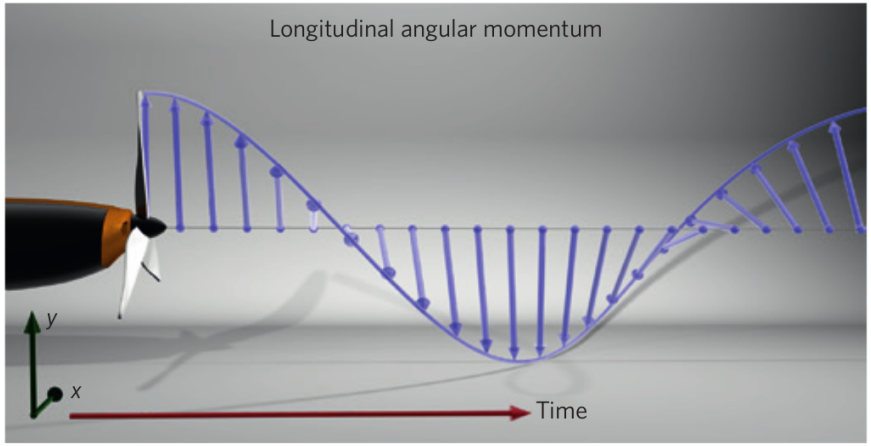


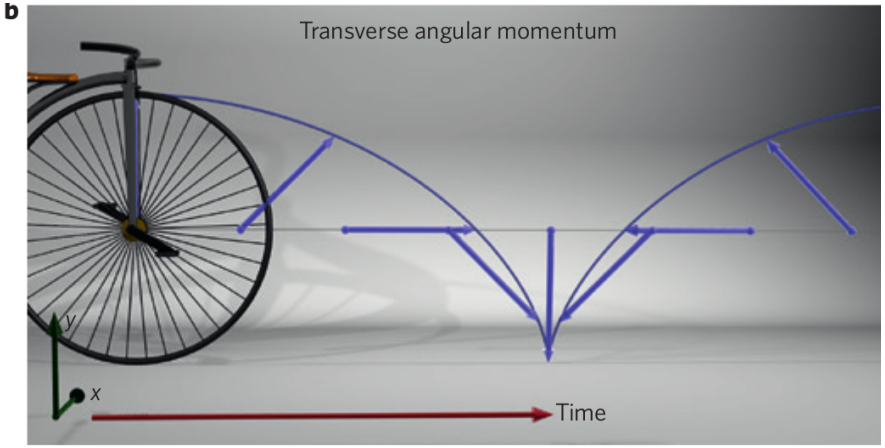
Profile of electric field





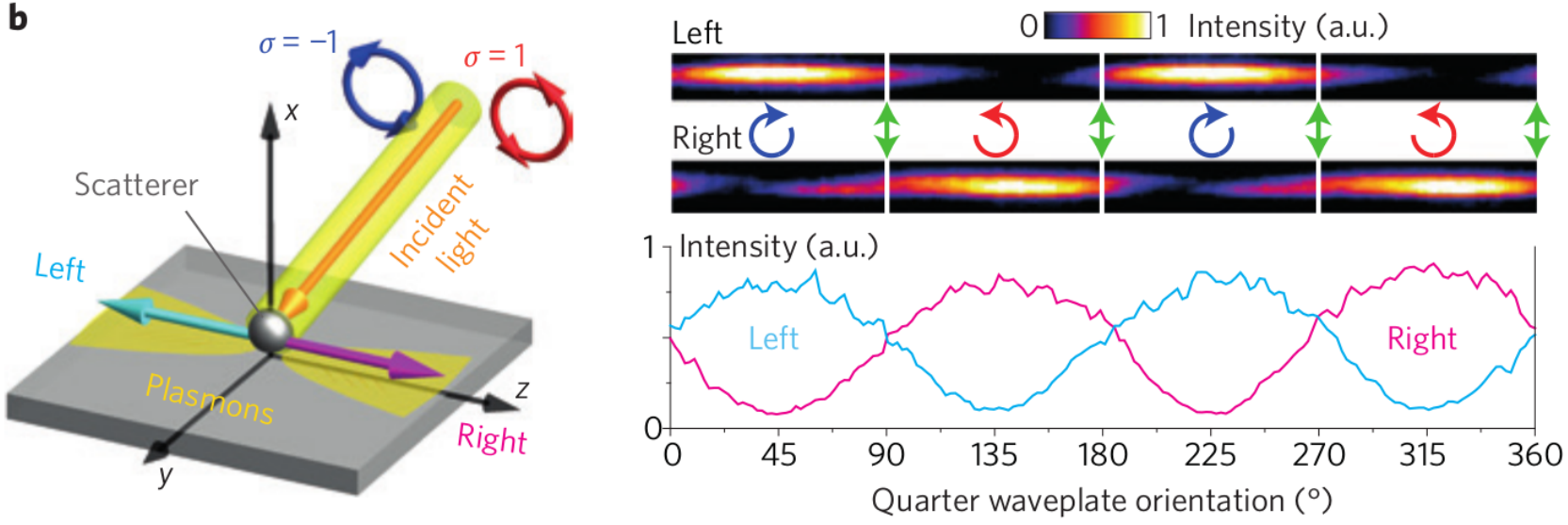
Profiles of electric field in paraxial beam and evanescent beam, providing longitudinal and transverse spin angular momentum.





Selection of evanescent wave propagation

As spin of the evanescent wave is given by propagation of spinwave, the polarization (helicity) of incoming beam determines propagation direction of the evanescent wave.



"Remarkably, the universal character of spin-direction locking in evanescent waves can be associated with the quantum spin-Hall effect of photons, which makes it an optical counterpart of the quantum spin-Hall effect of electrons in topological insulators"

Spin-orbit interaction

Spin-orbit coupling: Dirac equation

Spin-orbit coupling term couples spin of the electron $\boldsymbol{\sigma} = 2\mathbf{S}/\hbar$ with movement of the electron $m\mathbf{v} = \mathbf{p} - e\mathbf{A}$ in presence of electrical field $\mathbf{E}$.

$$H_{SOC} = -\frac{e\hbar}{4m^2c^2}\boldsymbol{\sigma} \cdot [\mathbf{E} \times (\mathbf{p} - e\mathbf{A})]$$

The maximal coupling is obtained when all three componets are perpendicular each other.
The spin-orbit term can be determined from solution of electron state in relativistic case. The equation describing relativistic electron is called Dirac equation, relativistic analogue of Schrodinger equation.

Dirac equation: introduction I

- Relativity describes nature at high speeds, $v \approx c$.
- Relativity unites time and space, described by Lorentz transformation

$$x' = \frac{x - vt}{\sqrt{1 - \frac{v^2}{c^2}}} \qquad t' = \frac{t - \frac{vx}{c^2}}{\sqrt{1 - \frac{v^2}{c^2}}}$$

$\Rightarrow$ relativistic quantum theory must do the same. Schrodinger equation does not fulfils this, as it it has first derivative in time and second in space.

Dirac equation: introduction II

Relativistic theory expresses total energy of the particle as:

$$W^2 = p^2c^2 + m_0^2c^4 \tag{3}$$

Quantum operator substitution: $\mathbf{p} \to \hat{\mathbf{p}} = -i\hbar\nabla$,
$W \to \hat{W} = i\hbar\partial/\partial t$. It follows in Klein-Gordon equation

$$\left(\nabla^2 - \frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \frac{m_0^2c^2}{\hbar^2}\right)\psi(\mathbf{r}, t) = 0 \tag{4}$$

This Eq. reduces to Eq. (3) for plane wave (free particle)
$\psi(\mathbf{r}, t) = \exp[i(\mathbf{r}\cdot\mathbf{p} - Wt)/\hbar]$. This condition limits following solutions to particles with spin $1/2$, as space-time wavefunction is symmetric, and hence spin-part must be antisymmetric.

Dirac equation: derivation I

1. let as ASSUME, the Dirac equation will have first derivative in time. Then, it must be also in first derivative in space.
2. wave function is superposition of N base wavefunctions $\psi(\mathbf{r}, t) = \sum \psi_n(\mathbf{r}, t)$
3. must fulfil Klein-Gordon equation, Eq. (4)

General expression of condition 1:

$$\frac{1}{c}\frac{\partial \psi_i(\mathbf{r}, t)}{\partial t} = -\sum_{w=x,y,z}\sum_{n=1}^{N} \alpha_{i,n}^{w}\frac{\partial \psi_n}{\partial w} - \frac{imc}{\hbar}\sum_{n=1}^{N}\beta_{i,n}\psi_n(\mathbf{r}, t) \quad (5)$$

Dirac equation: derivation II

When expressed in matrix form (ψ is column vector, $\alpha_{i,n}^{k}$ is $3 \times N \times N$ matrix, $\beta_{i,n}$ is $N \times N$ matrix)

$$\frac{1}{c}\frac{\partial \psi(\mathbf{r},t)}{\partial t} = -\tilde{\boldsymbol{\alpha}} \cdot \nabla \psi(\mathbf{r},t) - \frac{imc}{\hbar}\tilde{\beta}\psi(\mathbf{r},t) \tag{6}$$

Substituting quantum operators $\hat{\mathbf{p}} \to -i\hbar\nabla$, we get Dirac equation

$$i\hbar\frac{\partial \psi(\mathbf{r},t)}{\partial t} = \hat{H}\psi(\mathbf{r},t) = (c\tilde{\boldsymbol{\alpha}} \cdot \hat{\mathbf{p}} + \tilde{\beta}mc^2)\psi(\mathbf{r},t) \tag{7}$$

where matrices $\tilde{\alpha}$, $\tilde{\beta}$ are unknown.

Dirac equation: non-relativistic limit

When Dirac equation is solved up to order $1/c^2$, we get

$$\hat{H} = \frac{1}{2m}\left(\frac{\hbar}{i}\nabla - e\mathbf{A}(\mathbf{r})\right)^2 + V(\mathbf{r}) + mc^2 \qquad \text{Unrelativistic Hamiltonian}$$

$$- \frac{e\hbar}{2m}\boldsymbol{\sigma}\cdot\mathbf{B} \qquad \text{Zeeman term}$$

$$- \frac{e\hbar}{4m^2c^2}\boldsymbol{\sigma}\cdot[\mathbf{E}\times(\mathbf{p}-e\mathbf{A})] \qquad \text{Spin}-\text{orbit coupling}$$

$$- \frac{1}{8m^3c^2}(\mathbf{p}-e\mathbf{A})^4 \qquad \text{Mass of electron increases with speed}$$

$$+ \frac{\hbar^2 e}{8m^2c^2}\nabla^2 V(\mathbf{r}) \qquad \text{Darwin term}$$

Darwin term: electron is not a point particle, but spread in volume of size of Compton length $\approx \hbar/mc$.

Spin-orbit coupling: discussion I

Spin-orbit coupling term can be sepaarted into two components:

$$-\frac{e\hbar}{4m^2c^2}\boldsymbol{\sigma}\cdot[\mathbf{E}\times(\mathbf{p}-e\mathbf{A})] = -\frac{e\hbar}{4m^2c^2}\boldsymbol{\sigma}\cdot[\mathbf{E}\times\mathbf{p}] + \frac{e^2\hbar}{4m^2c^2}\boldsymbol{\sigma}\cdot[\mathbf{E}\times\mathbf{A}]$$
$$= H_{SOC} + H_{AME}$$

AME=Angular magneto-electric

- The electric field $\mathbf{E} = -\frac{1}{e}\nabla V - \frac{\partial}{\partial t}\mathbf{A}$
- canonical momentum $\mathbf{p} = -i\hbar\nabla$ (conjugate variable of position; $\frac{\partial H}{\partial x_i} = -\dot{p}_i$, $\frac{\partial H}{\partial p_i} = \dot{x}_i$)
- kinetical momentum $m\mathbf{v} = \mathbf{p} - e\mathbf{A}$ (defines kinetic energy and represents velocity)

H_{SOC} in spherical potential, static case

$$H_{SOC} = -\frac{e\hbar}{4m^2c^2}\boldsymbol{\sigma} \cdot [\mathbf{E} \times \mathbf{p}]$$

Spherical potential $V(\mathbf{r}) = V(|\mathbf{r}|) = V(r)$; static case $\frac{\partial}{\partial t}\mathbf{A} = 0$:

$$e\mathbf{E} = -\nabla V(|\mathbf{r}|) = \frac{dV(r)}{dr}\frac{\mathbf{r}}{|\mathbf{r}|}$$

providing:

$$H_{SOC} = \frac{\hbar}{4m^2c^2}\frac{1}{r}\frac{dV}{dr}\boldsymbol{\sigma} \cdot (\mathbf{r} \times \mathbf{p}) = \frac{1}{2m^2c^2}\frac{1}{r}\frac{dV}{dr}\mathbf{S} \cdot \mathbf{L} = \xi \mathbf{S} \cdot \mathbf{L}$$

where spin angular momentum $\mathbf{S} = \frac{\hbar}{2}\boldsymbol{\sigma}$ and orbital angular momentum $\mathbf{L} = \mathbf{r} \times \mathbf{p}$

Understanding spin-orbit coupling: spherical potential

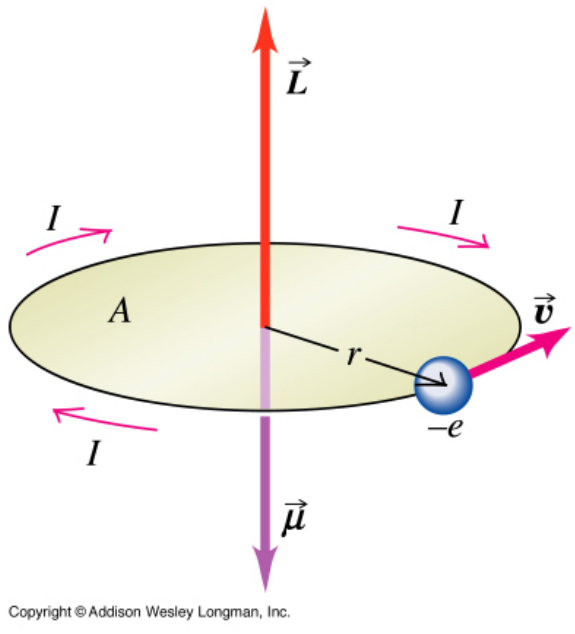
- spin of the electron creates electron's magnetic moment (in SI)

$$\boldsymbol{\mu}_S = -\frac{e}{m}\mathbf{S} = -\frac{e}{m}\frac{h}{2}\boldsymbol{\sigma} = -\mu_b\boldsymbol{\sigma} = -\frac{2\mu_B}{\hbar}\mathbf{S}$$

  where $\mu_B = \frac{e\hbar}{2m}$ is Bohr magneton.
- orbital moment (around atomic core) creates magnetic moment too

$$\boldsymbol{\mu}_L = -\frac{e}{2m}\mathbf{L} = -\frac{\mu_B}{\hbar}\mathbf{L} = -\mu_B l$$

  (or can be understood as creating magnetic field H_{eff} due to current created by electron orbital)
- the mutual static energy of spin and orbital is then $E_{SO,approx} = -\boldsymbol{\mu}_S \cdot \mathbf{B}_{eff}$ or just electrostatic interaction between both magnetic dipoles.



Understanding spin-orbit coupling: Lorentz transformation

Electromagnetic field appears different as observing frame is moved. For example, if a charge is moving in the laboratory frame (unprimed), we observe both electric and magnetic fields. In the frame of the moving charge (primed), only electric field is observed and the current and magnetic field are absent. Lorentz transformation of el.-mag. fields between both frames is:

$$\mathbf{E}'_{\parallel} = \mathbf{E}_{\parallel} \qquad \mathbf{B}'_{\parallel} = \mathbf{B}_{\parallel}$$

$$\mathbf{E}'_{\perp} = \frac{(\mathbf{E} + \mathbf{v} \times \mathbf{B})_{\perp}}{\sqrt{1 - \frac{v^2}{c^2}}} \qquad \mathbf{B}'_{\perp} = \frac{(\mathbf{B} - \mathbf{v}/c^2 \times \mathbf{E})_{\perp}}{\sqrt{1 - \frac{v^2}{c^2}}}$$

where $\perp$ and $\parallel$ are relative to the direction of the velocity $\mathbf{v}$.
I.e. for small speeds, $\mathbf{E}' = \mathbf{E} + \mathbf{v} \times \mathbf{B}$ and $\mathbf{B}' = \mathbf{B} - \frac{\mathbf{v}}{c^2} \times \mathbf{E}$

Understanding spin-orbit coupling: Lorentz transformation

For electron flying by speed $\mathbf{v}$ through static electric field $\mathbf{E}$, in its frame the electron feels magnetic field $\mathbf{B}' = -\frac{-\mathbf{v}}{c^2} \times \mathbf{E}$, which torques/acts on its spin. The Hamiltonian is given by Zeeman interaction

$$H_{SO,E\to B} = -\boldsymbol{\mu}_S \cdot \mathbf{B}' \tag{8}$$

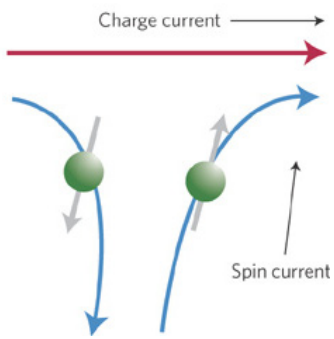
$$= -\left(-\frac{e\hbar}{2m}\boldsymbol{\sigma}\right) \cdot \left(-\frac{1}{c^2}(-\mathbf{v}) \times \mathbf{E}\right) \tag{9}$$

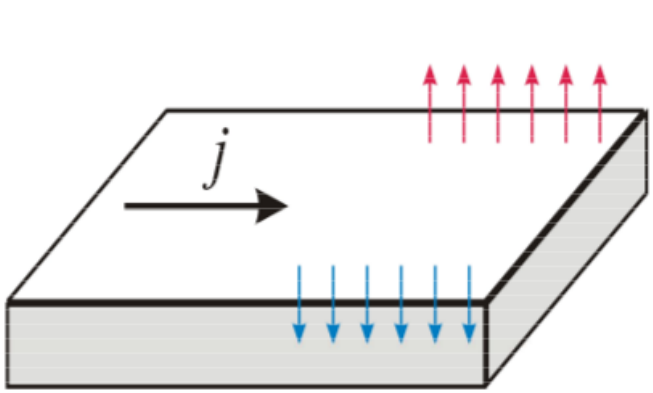
$$= -\frac{e\hbar}{2m^2c^2}\boldsymbol{\sigma} \cdot (\mathbf{E} \times \mathbf{p}) \tag{10}$$

which is twice larger compared to H_{SOC} derived from Dirac equation. Missing half is due to Thomas precession (in case of electron orbiting nucleus, it is the precession of the electron rest frame as it orbits around the nucleus).

Lorentz transformation: extrinsic spin Hall effect

In laboratory frame, spin-Hall effect provides scattering of electrons on charged impurity along to electron spin.
In electron frame, it can be understood as charge current from impurities, providing magnetic field, according which the electron spin aligns.





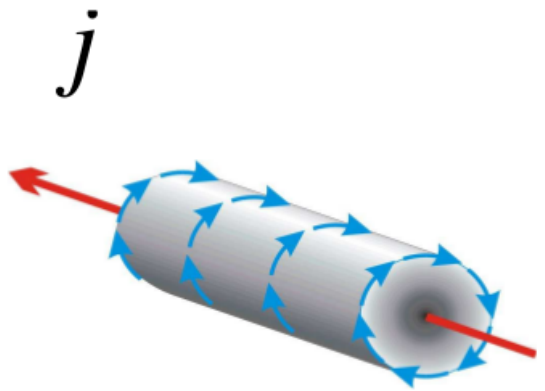


Figure 1. The Spin Hall Effect. An electrical current induces spin accumulation at the lateral boundaries of the sample. In a cylindrical wire the spins wind around the surface, like the lines of the magnetic field produced by the current. However the value of the spin polarization is much greater than the (usually negligible) equilibrium spin polarization in this magnetic field.

Examples of spin-orbit effects

$$H_{SOC} = -\frac{e\hbar}{4m^2c^2}\boldsymbol{\sigma} \cdot [\mathbf{E} \times (\mathbf{p} - e\mathbf{A})]$$

Various SOC effects are obtained by different origins of $\mathbf{A}$ and $\mathbf{E} = \frac{1}{e}\nabla V - \frac{\partial}{\partial t}\mathbf{A}$.
Examples:

- SOC in spherical potential (already discussed)
- optical spin pumping: excitation of electrons with selective spins in GaAs
- $\mathbf{E}$ has contribution originating from interface of two materials: $\rightarrow$ Rasha effect
- $\mathbf{A}$ has contribution of incident light: coupling between angular momentum of light and electron spin (optomagnetic field)

Example: splitting of atomic levels by SOC

Splitting of atomic levels due to spin-orbit coupling (without magnetic field). The energy levels corresponds to different values of the total angular momentum **J**

$$\mathbf{J} = \mathbf{L} + \mathbf{S}$$

$$\mathbf{J} \cdot \mathbf{J} = (\mathbf{L} + \mathbf{S}) \cdot (\mathbf{L} + \mathbf{S}) = \mathbf{L} \cdot \mathbf{L} + \mathbf{S} \cdot \mathbf{S} + 2 \langle \mathbf{L} \cdot \mathbf{S} \rangle$$

$$j(j+1) = l(l+1) + s(s+1) + 2 \langle \mathbf{L} \cdot \mathbf{S} \rangle$$

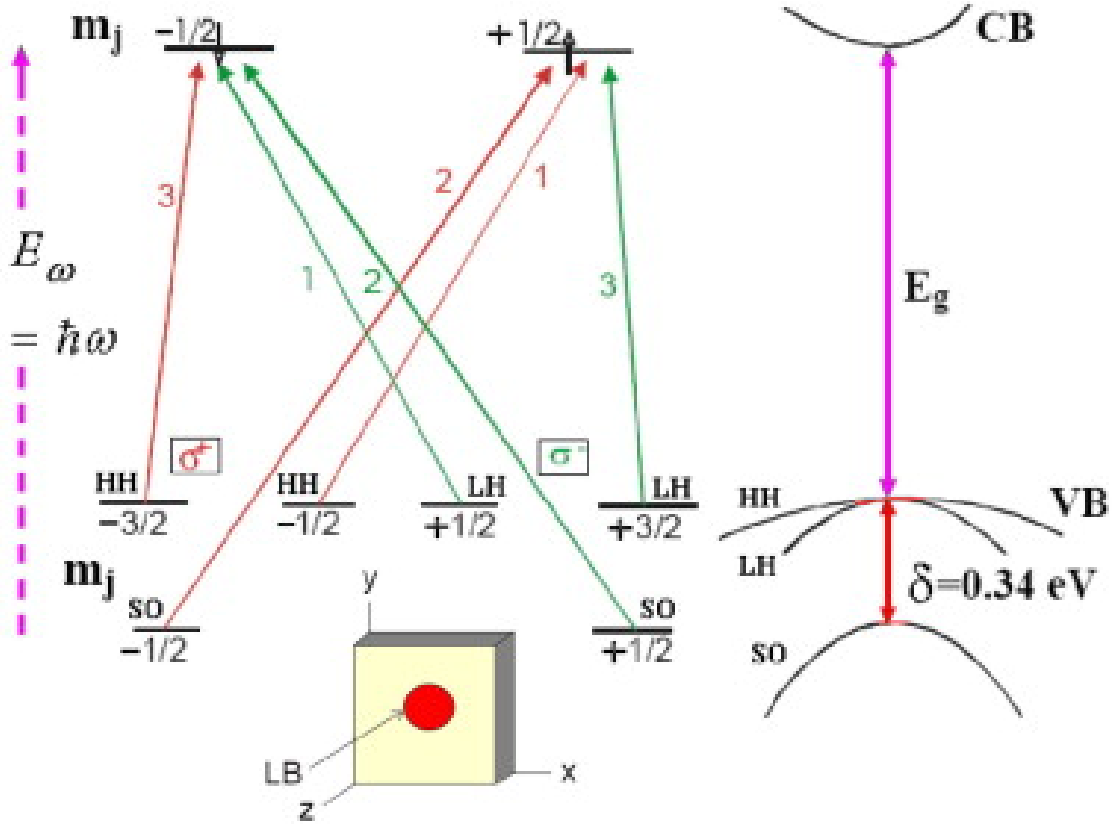
$$\langle \mathbf{L} \cdot \mathbf{S} \rangle = \frac{1}{2} \left[j(j+1) - l(l+1) - s(s+1) \right]$$

For p states, $l = 1$, $s = 1/2$ and $j = 3/2$ (4 electrons) or $1/2$ (2 electrons). So, due to spin-orbit coupling (without magnetic field), the energy level of electron splits into two levels.
Thus, the spin-orbit interaction does not lift all the degeneracy for atomic states. To lift this additional degeneracy it is necessary to apply a magnetic field.

Optical spin orientation

Electron excitation by circularly polarized beam in GaAs excites electrons with selective spins.

- for $\hbar\omega$ between E_g and $E_g + \Delta_{SO}$, only the light and heavy hole subband are excited. Then for zinc-bland structure (e.g. GaAs), the spin-polarization is $P_n = -1/2$.
- Light polarization can also be used to detect spin polarization in semiconductors.

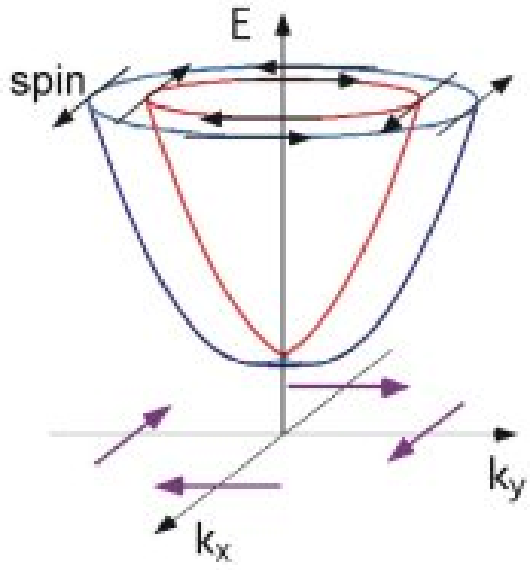


Rashba effect I

Rashba Hamiltonian: electric field **E** is created on interface, $\mathbf{E} \parallel \hat{z}$:

$$H_{\text{Rashba}} = \alpha(\boldsymbol{\sigma} \times \mathbf{p}) \cdot \hat{\mathbf{z}}$$

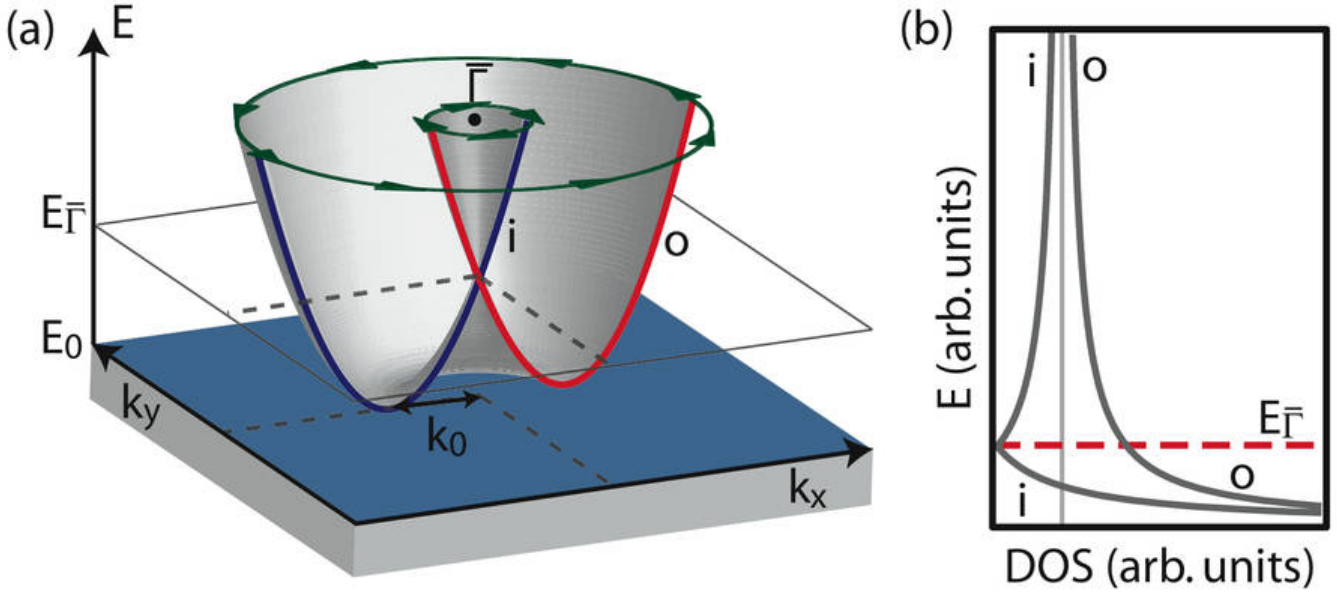
α: Rasba coupling
p: electron's momentum
σ: spin direction (Pauli matrix vector)



The Rashba effect is a momentum dependent splitting of spin bands in two-dimensional condensed matter systems (heterostructures and surface states). It originates from concurrent appearance of

- spin-orbit coupling
- asymmetry of the potential in the direction $\hat{z}$ perpendicular to the two-dimensional plane, creating electric field $\mathbf{E} = E_z\hat{z} = -\frac{1}{e}\nabla V$

Rashba effect II



http://www.sps.ch/fr/articles/progresses/

- For $\mathbf{p} = p_x$ and $H_{\text{Rashba}} = \alpha(\boldsymbol{\sigma} \times \mathbf{p}) \cdot \hat{z} \Rightarrow H_{\text{Rashba}} = -\alpha p_x \sigma_y$
- splitting of energy states according to $\mathbf{p}$ and $\boldsymbol{\sigma}$ directions.
- max. splitting when z, $\mathbf{p}$ and $\boldsymbol{\sigma}$ are perpendicular each other.
- when crystal lacks inversion symmetry, internal electric field $\mathbf{E}$ is created.

Optomagnetic field I

according to: Paillard, Proc. of SPIE 9931, 99312E-1 (2016)

$$H_{AME} = -\frac{e^2\hbar}{4m^2c^2}\boldsymbol{\sigma}\cdot[\mathbf{E}\times\mathbf{A}]$$

Assume electric field as plane wave

$$\mathbf{E}_{\text{ext}} = -\frac{\partial\mathbf{A}}{\partial t} = \Re\left(\mathbf{E}_0\exp[i(\mathbf{k}\cdot\mathbf{r}-\omega t)]\right)$$

providing vector potential as $\mathbf{A} = \Re(-\frac{i}{\omega}\mathbf{E}_0\exp[i(\mathbf{k}\cdot\mathbf{r}-\omega t)])$

- Electric field acting on electron has two contributions, $\mathbf{E} = \mathbf{E}_{\text{int}} + \mathbf{E}_{\text{ext}}$, $\mathbf{E}_{\text{int}} = -1/e\nabla V$ provided by crystal and $\mathbf{E}_{\text{ext}}$ provided by incoming el.-mag. field.
- term $[\mathbf{E}_{\text{int}}\times\mathbf{A}]$ vanishes as $\mathbf{E}_{\text{int}}$ varies much quicker compared to $\mathbf{A}$ (due to $a \ll \lambda$).

Optomagnetic field II

$$H_{AME} = -\frac{e^2\hbar}{8m^2c^2\omega}\boldsymbol{\sigma}\cdot\Re[i\mathbf{E}_0\times\mathbf{E}_0^*] = -\boldsymbol{\mu}_B\cdot\mathbf{B}_{OM}$$

$$\mathbf{B}_{OM} = -\frac{\mu_B}{\varepsilon_0 c^3\omega\hbar}I\boldsymbol{\sigma}_{\text{helicity}}$$

- $\boldsymbol{\mu} = -\mu_b\boldsymbol{\sigma}$: electron magnetic moment, $\mu_b = e\hbar/(2m)$ Bohr magneton
- $\boldsymbol{\sigma}_{\text{helicity}} = \Re[i\mathbf{u}\times\mathbf{u}]$: helicity of beam, where $\mathbf{u}$ is beam polarization, $\mathbf{u} = \mathbf{E}_0/E_0$
- $I = \frac{c\varepsilon_0}{2}E_0^2$: beam intensity
- direction of $\mathbf{B}_{OM}$ is determined by helicity of the incident beam $\boldsymbol{\sigma}_{\text{helicity}}$

Note: although $\mathbf{B}_{OM}$ contributes to magnetization torque by induced light, it is not probably the dominanting term.