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:

$$W^2 = p^2c^2 + m_0^2c^4 \tag{1}$$

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

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

This Eq. reduces to Eq. (1) 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. (2)

General expression of condition 1:

$$\frac{1}{c}\frac{\partial \psi_i(\mathbf{r},t)}{\partial t} = -\sum_{w=x,y,z}\sum_{n=1}^{N}\alpha_{i,n}^{w}\frac{\partial \psi_n}{\partial w} - \frac{imc}{\hbar}\sum_{n=1}^{N}\beta_{i,n}\psi_n(\mathbf{r},t) \quad (3)$$

Dirac equation: derivation II

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

$$\frac{1}{c}\frac{\partial \psi(\mathbf{r},t)}{\partial t} = -\tilde{\boldsymbol{\alpha}} \cdot \nabla \psi(\mathbf{r},t) - \frac{imc}{\hbar}\tilde{\beta}\psi(\mathbf{r},t) \tag{4}$$

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

$$i\hbar\frac{\partial \psi(\mathbf{r},t)}{\partial t} = \hat{H}\psi(\mathbf{r},t) = (c\tilde{\boldsymbol{\alpha}} \cdot \hat{\mathbf{p}} + \tilde{\beta}mc^2)\psi(\mathbf{r},t) \tag{5}$$

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

$$
\begin{aligned}
\hat{H} =& \frac{1}{2m}\left(\frac{\hbar}{i}\nabla - e\mathbf{A}(\mathbf{r})\right)^2 + V(\mathbf{r}) + mc^2 \qquad \text{Unrelativistic Hamiltonian} \\
& - \frac{e\hbar}{2m}\boldsymbol{\sigma}\cdot\mathbf{B} \qquad \text{Zeeman term} \\
& - \frac{e\hbar}{4m^2c^2}\boldsymbol{\sigma}\cdot[\mathbf{E}\times(\mathbf{p} - e\mathbf{A})] \qquad \text{Spin-orbit coupling} \\
& - \frac{1}{8m^3c^2}(\mathbf{p} - e\mathbf{A})^4 \qquad \text{Mass of electron increases with speed} \\
& + \frac{\hbar^2 e}{8m^2c^2}\nabla^2 V(\mathbf{r}) \qquad \text{Darwin term}
\end{aligned}
$$

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

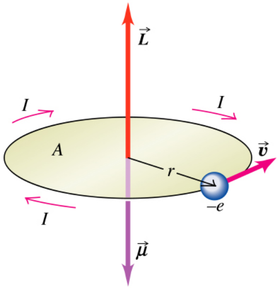
- spin of the electron creates electron's magnetic moment (in SI)

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

  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

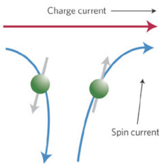
For electron flying by speed $\mathbf{v}$ through static electric field $\mathbf{E}$, in its frame the electron feels magnetic field $\mathbf{B}' = -\frac{-\mathbf{v}}{c^2} \times \mathbf{E}$, which torques/acts on its spin. The Hamiltonian is given by Zeeman interaction

$$
\begin{aligned}
H_{SO,E\to B} &= -\boldsymbol{\mu}_S \cdot \mathbf{B}' && (6)\\
&= -\left(-\frac{e\hbar}{2m}\boldsymbol{\sigma}\right) \cdot \left(-\frac{1}{c^2}(-\mathbf{v}) \times \mathbf{E}\right) && (7)\\
&= -\frac{e\hbar}{2m^2c^2}\boldsymbol{\sigma} \cdot (\mathbf{E} \times \mathbf{p}) && (8)
\end{aligned}
$$

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.



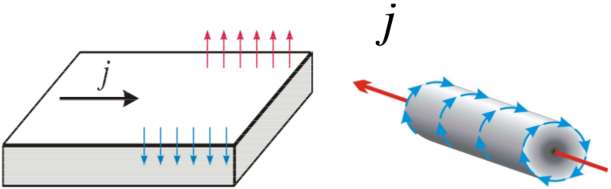


Figure 1. The Spin Hall Effect. An electrical current induces spin accumulation at the lateral boundaries of the sample. In a cylindrical wire the spins wind around the surface, like the lines of the magnetic field produced by the current. However the value of the spin polarization is much greater than 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 **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
- **E** has contribution originating from interface of two materials: $\rightarrow$ Rasha effect
- **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**

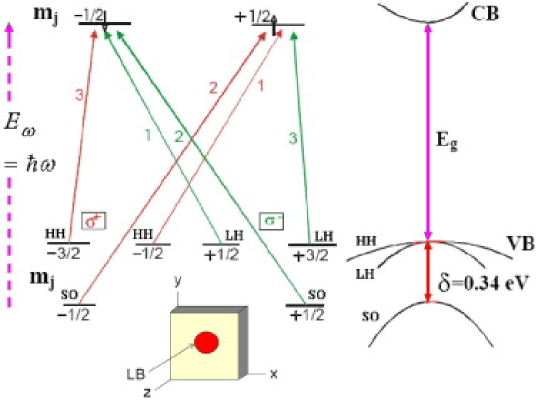
$$\mathbf{J} = \mathbf{L} + \mathbf{S}$$
$$\mathbf{J} \cdot \mathbf{J} = (\mathbf{L} + \mathbf{S}) \cdot (\mathbf{L} + \mathbf{S}) = \mathbf{L} \cdot \mathbf{L} + \mathbf{S} \cdot \mathbf{S} + 2 \langle \mathbf{L} \cdot \mathbf{S} \rangle$$
$$j(j+1) = l(l+1) + s(s+1) + 2 \langle \mathbf{L} \cdot \mathbf{S}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

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.

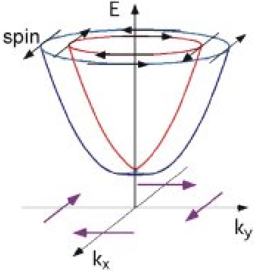


Rashba effect I

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

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

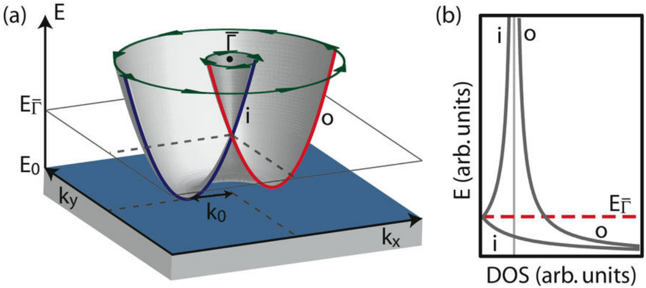
α: Rasba coupling
p: electron's momentum
σ: spin direction (Pauli matrix vector)



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 **p** and $\boldsymbol{\sigma}$ directions.
- max. splitting when z, **p** and $\boldsymbol{\sigma}$ are perpendicular each other.
- when crystal lacks inversion symmetry, internal electric field **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

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

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, $\mathbf{E} = \mathbf{E}_{\rm int} + \mathbf{E}_{\rm ext}$, $\mathbf{E}_{\rm int} = -1/e\nabla V$ provided by crystal and $\mathbf{E}_{\rm ext}$ provided by incoming el.-mag. field.
- term $[\mathbf{E}_{\rm int}\times\mathbf{A}]$ vanishes as $\mathbf{E}_{\rm int}$ 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.