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# *10TH CONFERENCE ON HOPPING AND RELATED PHENOMENA*

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# *"Spin Transport in Two-Dimensional Hopping Systems"*

presented by:

**T. DAMKER**
Otto-von-Guericke Universität
Magdeburg
Germany

# Spin Transport in Two-Dimensional Hopping Systems

Thomas Damker and Harald Böttger
Magdeburg, Germany

Valerii Bryksin
St. Petersburg, Russia

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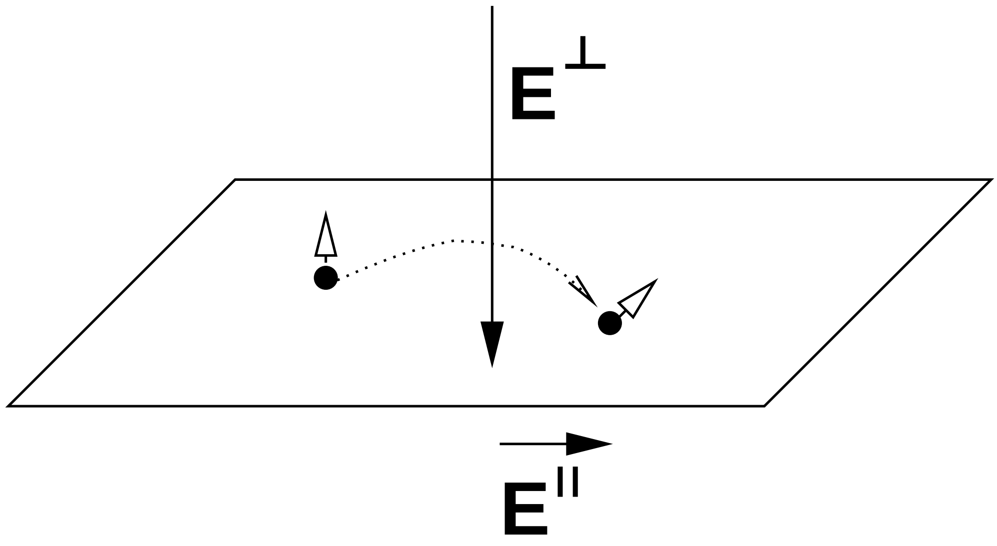
- Motivation
- Model and Procedure
- Spin-Polarization
- Summary and Outlook

# Motivation

- **Spintronics**
  - utilize spin degree of freedom "technologically" (spin transistor)
  - influence spin with electrical means
  - interplay between spin and charge transport
- **anomalous Hall effect**
  spin polarized electrons $\rightarrow$ anisotropic charge transport
- **Spin-Hall effect**
  - spin accumulation
  - non-equilibrium spin distribution (spin polarization) due to electric field (no magnetic field or material)
- **Aim:** to consider spin transport in hopping conduction

# The Model




- electrons confined to **2D plane**
  (e.g. heterostructure, organic semiconductor)

- electronic states **localized**
  (e.g. disorder, polaron formation)

- large perpendicular electric field $\vec{E}^{\perp}$ ($\propto \vec{K}$)
  (e.g. due to heterostructure confinement field, can be modified by a gate voltage)
  $\rightarrow$ **Rashba spin-orbit interaction** (SOI)

- in-plane field $\vec{E}^{||}$
  $\rightarrow$ induces current in plane

- center of interest: evolution of **spin** degree of freedom

# Procedure

- include Rashba-SOI into hopping formalism
  → SU(2) "phase factor" (cf. Holstein transformation)

$$J^{\mathrm{SO}}_{m'm} = e^{-i\vec{\sigma}\cdot(\vec{K}\times\vec{R}_{m'm})} J_{m'm}$$

- Konstantinov-Perel diagram technique
  (first step: second-order diagrams in one-particle approximation)
- rate equations for generalized occupation probability ($2 \times 2$-matrix)

$$\hat{\rho}_m|_{\sigma'\sigma} = \langle a^{\dagger}_{m\sigma'} a_{m\sigma} \rangle$$

- rate equations for
  - $\rho_m = \mathrm{Tr}(\hat{\rho}_m)$ — occupation probability
  - $\vec{\rho}_m = \mathrm{Tr}(\vec{\sigma}\hat{\rho}_m)$ — spin orientation
- ordered 2d system
  → solution in wave vector space
- back-transformation to time and space co-ordinates

# Spin-Orbit Interaction (SOI)

Dirac equation $\rightarrow$ series up to terms of order $1/c^2$

$$
\begin{aligned}
H \quad = \quad & \frac{1}{2m}\left(\mathbf{p} - \frac{e}{c}\mathbf{A}\right)^2 + e\phi - \frac{e\hbar}{2mc}\boldsymbol{\sigma} \cdot \mathrm{rot}\mathbf{A} \\
& -\frac{\mathbf{p}^4}{8m^3c^2} \quad \text{relativistic contribution to kinetic energy} \\
& +\frac{e\hbar}{4m^2c^2}\boldsymbol{\sigma} \cdot ((\boldsymbol{\nabla}\phi) \times \mathbf{p}) \quad \text{spin-orbit interaction} \\
& +\frac{e\hbar^2}{8m^2c^2}\Delta\phi \quad \text{Darwin term}
\end{aligned}
$$

Darwin term: “zitterbewegung” of the electron over a spatial distance of the order of the Compton length
$\langle V(x)\rangle \approx V(x) + \langle \delta x^2 \rangle \Delta V(x)/2$
$\rightarrow$ can be absorbed into one-particle potential

spin operator $\mathbf{S} = \hbar\boldsymbol{\sigma}/2$
magnetic field $\mathbf{B} = \mathrm{rot}\mathbf{A}$
electric field $\mathbf{E} = -\boldsymbol{\nabla}\phi - \dot{\mathbf{A}}/c$

no magnetic field: $\mathbf{A} = 0$
homogeneous electric field: $\phi = -\mathbf{E} \cdot \mathbf{r}$
nonrelativistic motion: $v \ll c$

# Rashba-SOI

- $$H = \frac{1}{2m}\vec{p}^{\,2} + V(\vec{r}) - \frac{e\hbar}{4m^2c^2}\vec{\sigma}\cdot(\vec{E}\times\vec{p})$$

- abbreviation:

$$\vec{K} = \frac{e}{4mc^2}\vec{E} \qquad \left(+\frac{m}{\hbar^2}\alpha\vec{n}\right)$$

  - dimension of inverse length
  - corresponds to length over which electron has to be moved to invert spin orientation

- Hopping Hamiltonian

$$H = \sum_{m\sigma} \epsilon_m a^\dagger_{m\sigma} a_{m\sigma} + \sum_{mm'\sigma\sigma'} J^{m\sigma}_{m'\sigma'} a^\dagger_{m\sigma} a_{m'\sigma'}$$
$$+ \text{phonon terms}$$

- transition matrix element with SOI (condition $|\vec{K}\times\vec{R}| \ll 1$)

$$J^{\mathrm{SO}}_{m'm} = e^{-i\vec{\sigma}\cdot(\vec{K}\times\vec{R}_{m'm})} J_{m'm}$$

# Rate Equations

- density matrix $\langle a^\dagger_{m'\sigma'} a_{m\sigma} \rangle$
  - diagonal in space indices
  - **not** diagonal in spin indices
- $2 \times 2$-matrix $\hat{\rho}_m|_{\sigma'\sigma} = \langle a^\dagger_{m\sigma'} a_{m\sigma} \rangle$
  instead of occupation probability $\langle a^\dagger_m a_m \rangle$ on site $m$
- rate equations

$$\begin{aligned} s\hat{\rho}_m(s) &= \hat{\rho}_m|_0 \qquad \text{(initial conditions)} \\ +\sum_{m_1} &\Big\{ \; e^{-i\vec{\sigma}\cdot(\vec{K}\times\vec{R}_{m_1 m})}\hat{\rho}_{m_1}(s) e^{i\vec{\sigma}\cdot(\vec{K}\times\vec{R}_{m_1 m})} W_{m_1 m} \\ &\qquad -\hat{\rho}_m(s) W_{m m_1} \Big\} \end{aligned}$$

- occupation probability $\rho_m = \mathrm{Tr}(\hat{\rho}_m)$

$$s\rho_m = \rho_m|_0 + \sum_{m_1} \{\rho_{m_1} W_{m_1 m} - \rho_m W_{m m_1}\}$$

- spatial vector of the spin orientation $\vec{\rho}_m = \mathrm{Tr}(\vec{\sigma}\hat{\rho}_m)$

$$s\vec{\rho}_m = \vec{\rho}_m|_0 + \sum_{m_1} \{\mathrm{D}_{m_1 m}\vec{\rho}_{m_1} W_{m_1 m} - \vec{\rho}_m W_{m m_1}\}$$

# Ordered 2D System

- transition probability in wave-vector space

$$W(\vec{q}) = W(0) - \vec{q}^{\,2} D - i\mu \vec{q} \cdot \vec{E}$$

$D$ — diffusion constant
$\mu$ — mobility

- dimensionless units

$$\vec{x} = K\vec{r}, \qquad \tau = DK^2 t, \qquad \vec{\epsilon} = \frac{\mu}{DK}\vec{E}^{\parallel}$$

# Total Spin Polarization

- easy to calculate: $\vec{q} = 0$ expressions
- independent of spatial variation of initial conditions (only $\vec{\rho}_0(\vec{q} = 0)$ relevant)
- $\epsilon = 0$: relaxation

$$\rho^{\perp}(\tau) = e^{-8\tau}\rho_0^{\perp}, \qquad \vec{\rho}^{||}(\tau) = e^{-4\tau}\vec{\rho}_0^{||}$$

- $\epsilon \neq 0, \quad \vec{\rho}_0 = \vec{e}_z$: relaxation and oscillation

$$\rho^{\perp}(\tau) = e^{-6\tau}\left[\cos(2\tau\sqrt{\epsilon^2 - 1}) - \frac{\sin(2\tau\sqrt{\epsilon^2 - 1})}{\sqrt{\epsilon^2 - 1}}\right]$$

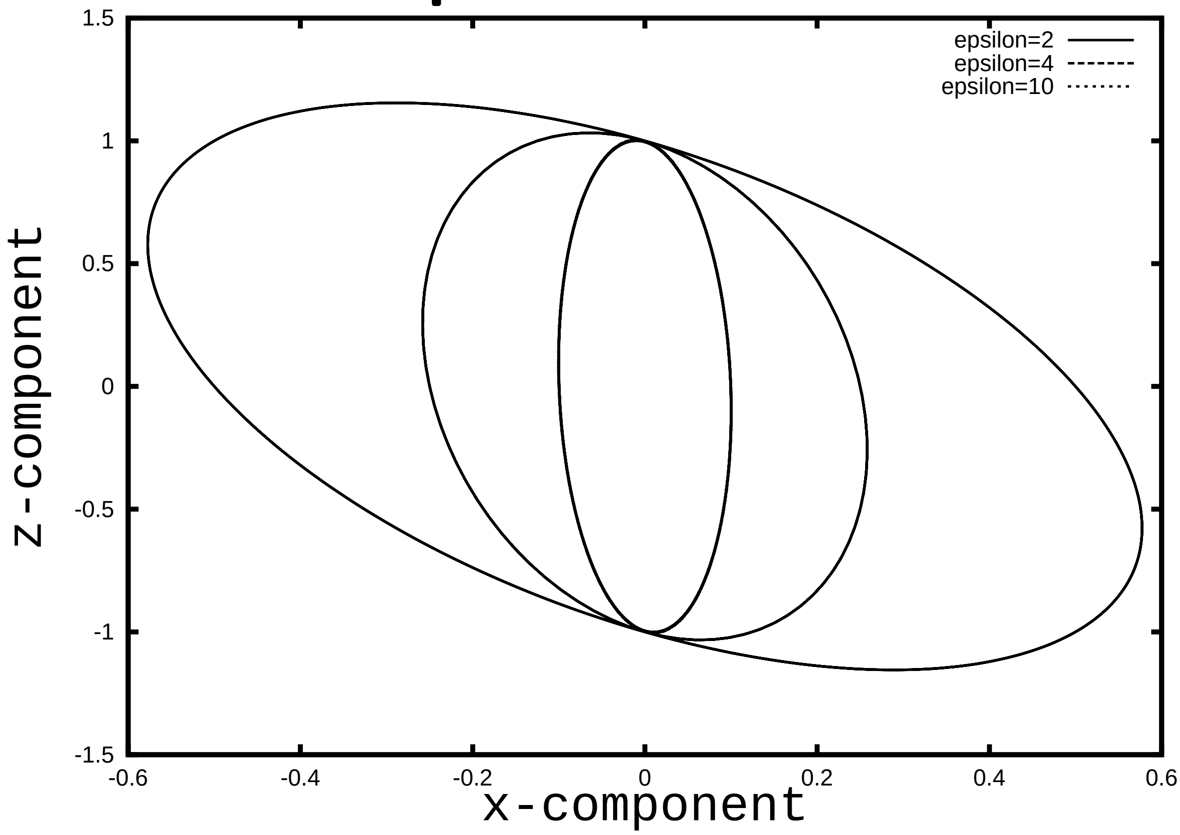
$$\vec{\rho}^{||}(\tau) = e^{-6\tau}\frac{\sin(2\tau\sqrt{\epsilon^2 - 1})}{\sqrt{\epsilon^2 - 1}}\vec{\epsilon}$$

- critical electric field $\epsilon_c = 1$:
  when $\epsilon < 1$, trigonometric functions become hyperbolic functions $\rightarrow$ exponential relaxation

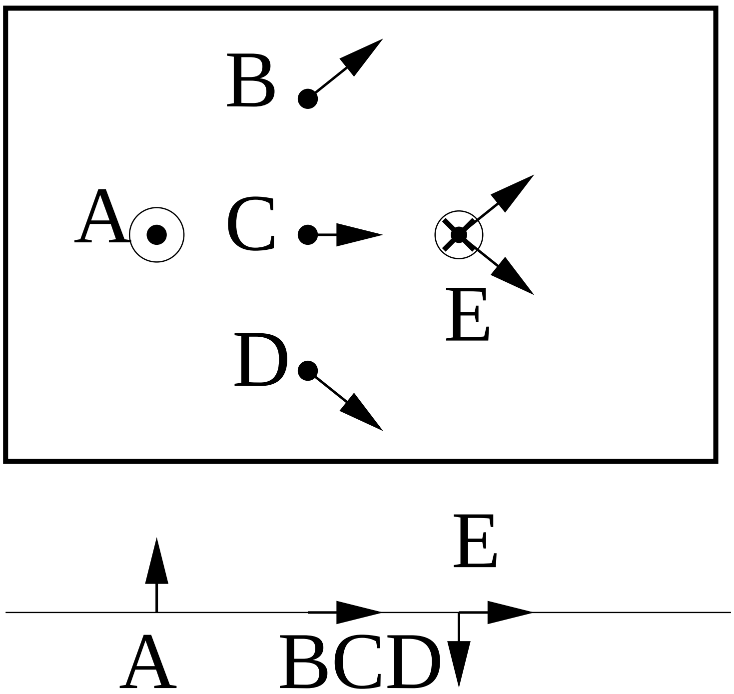
$$E_c^{||} = \frac{D}{4mc^2\mu}E^{\perp} = \frac{k_B T}{4mc^2}E^{\perp}$$

$\vec{\rho}(\tau)$

# Total Spin Polarization




# Graphic Explanation of Relaxation

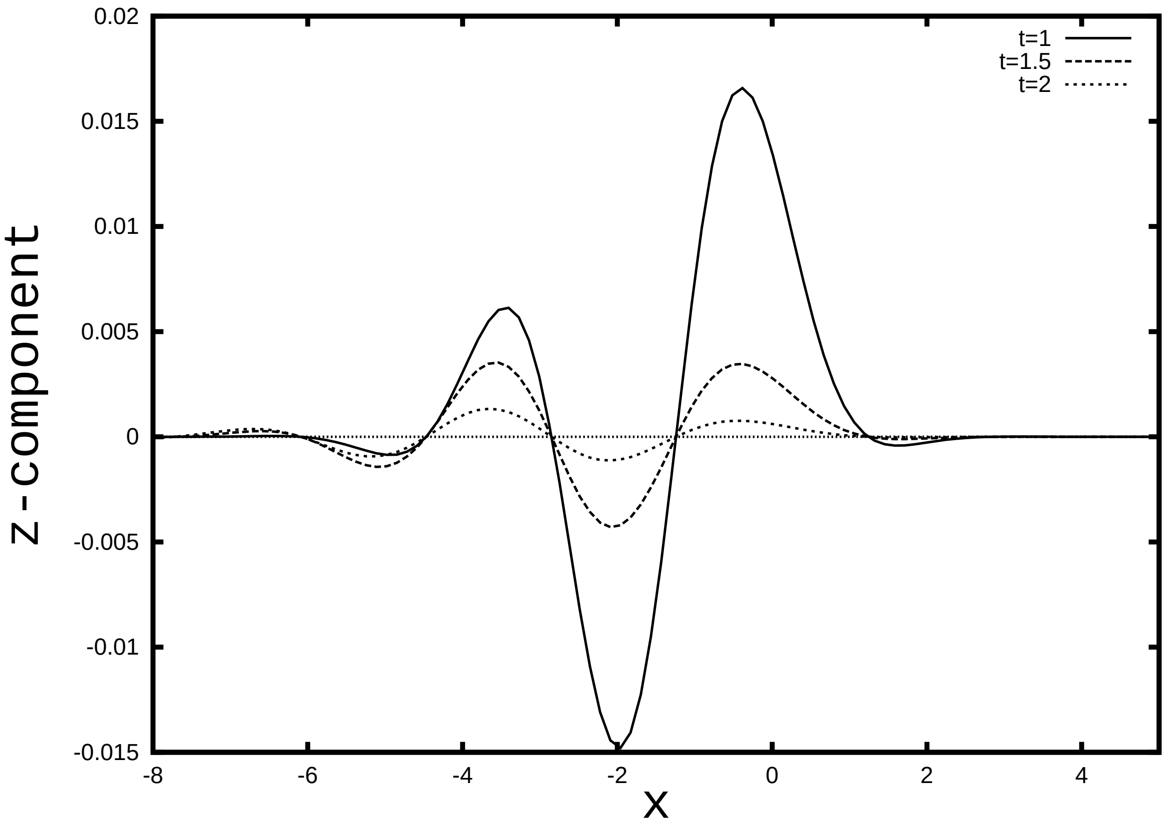


# Inhomogeneous Initial Conditions

- initial condition: $\vec{\rho}_0(\vec{x}) = \delta(\vec{x})\vec{e}_z$
- asymptotic term for $\tau \to \infty$ and $x \ll 2\sqrt{\tau}$:

$$\rho^{\perp}(\tau, \vec{x}) = e^{-\frac{\vec{\epsilon}\cdot\vec{x}}{2} - \frac{\epsilon^2\tau}{4} - \frac{7}{4}\tau - \frac{x^2}{4\tau}} \frac{3}{8\sqrt{\pi\tau}} \mathrm{J}_0\left(\frac{\sqrt{15}}{2}x\right)$$

- sign of $\rho^{\perp}$ at any fixed place is **not** time-dependent



# Low Symmetry

- $W(\vec{q})$ can be **anisotopic** in $\vec{q}$
- can lead to anisotropic charge transport
  (but still not spin dependent
  $\rightarrow$ no anomalous Hall effect)
- $$s\rho_m = \rho_m|_0 + \sum_{m_1} \{\rho_{m_1} W_{m_1 m} - \rho_m W_{m m_1}\}$$
- the quantitiy $D$ couples anisotropies of $W$ to changes in spin orientation
- $$s\vec{\rho}_m = \vec{\rho}_m|_0 + \sum_{m_1} \{\mathrm{D}_{m_1 m} \vec{\rho}_{m_1} W_{m_1 m} - \vec{\rho}_m W_{m m_1}\}$$
- spacial spin separation is possible
  $\rightarrow$ **spin Hall effect**

# Experimental Conditions

- Rashba SOI strength $\alpha \approx \underline{10^{-8}} \ldots 10^{-9}$ eV cm
  corresponds to $E^{\perp} \approx 2.7\ 10^{13}$ V/m $\times \left(\frac{m}{m_e}\right)^2$
  can be changed by applying a gate voltage (50%)
- inverse length scale for spin variations
  $K \approx \frac{m}{m_e} 1/76$ nm
- conditions for applicability:
  - $R_{m_1 m} \ll 1/K \approx 760$ Å
  - Rashba field yields largest contribution to spin dynamics
- critical field $E_c^{\|} \approx \left(\frac{m}{m_e}\right)^2 10^3$ V/m

# Summary

- **spin transport** for hopping electrons with Rashba-SOI
- charge transport is spin-independent in second-order theory
- **relaxation** of spin component perpendicular to plane is faster than in-plane spin relaxation
- **critical field** for transition between **oscillatory** and **exponential** behaviour of total spin polarisation
- spatial distribution of sign of spin projection is **time-independent**
- **spin separation** for low symmetry already in second-order theory

# Outlook

- third-order diagrams: spin dependent charge transport
- spatial disorder
- soften one-electron approximation (Pauli blocking, linear response)