Real-space distribution of the Hall current densities and their spin polarization in non-magnetic zinc-blende semiconductors

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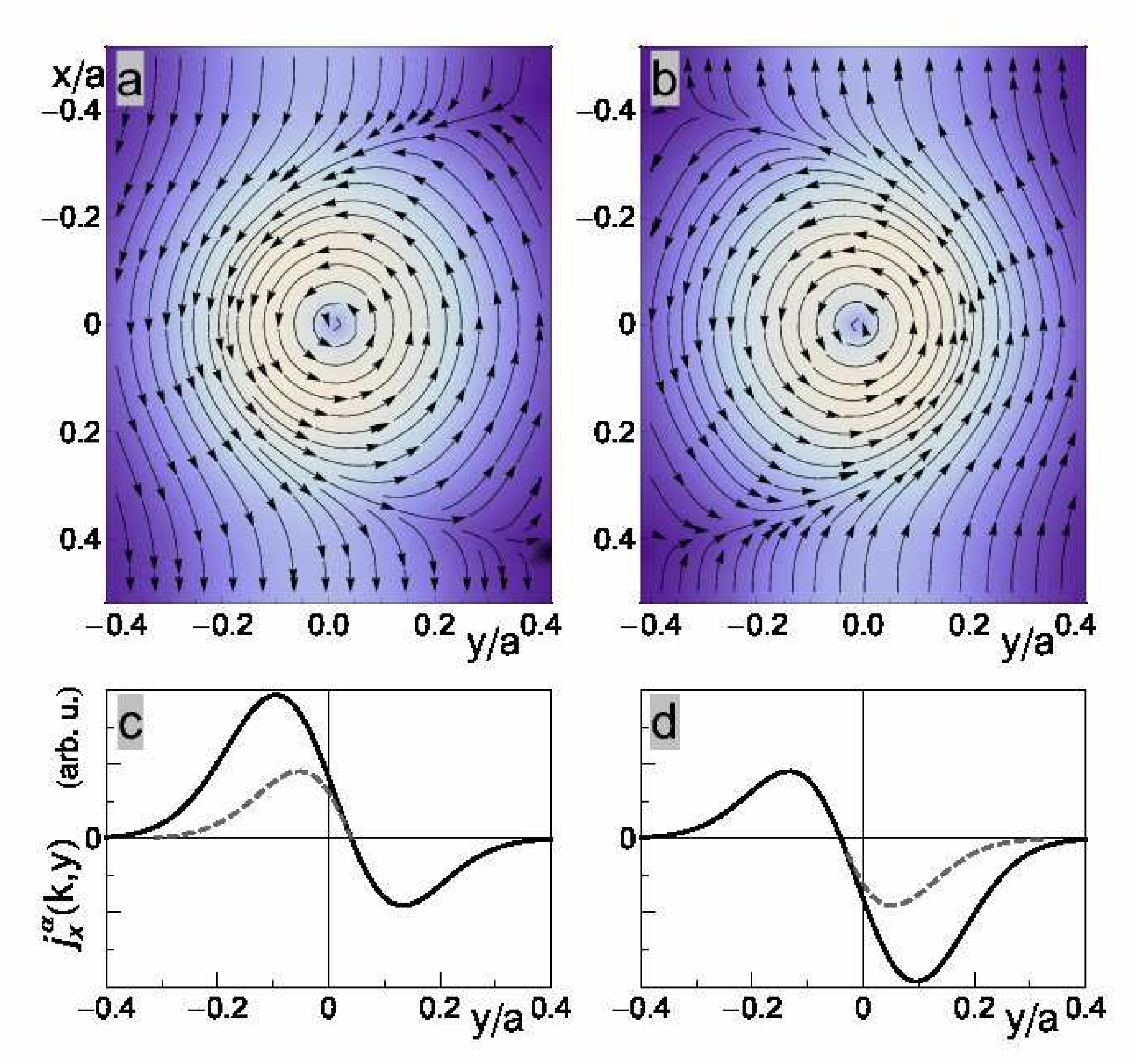
MOTIVATION

- non-magnetic semiconductors with zinc-blende structure are important materials used in spintronics
  - spin-orbit interaction leads to splitting of states, but
  - in equilibrium the total spin in any point of real space is zero (Kramer's theorem)
  - however, in non-equilibrium state spin polarization and spin-Hall current may appear
- spin-current operator is usually defined as a symmetrized product $\vec{j} = \frac{1}{2}[\sigma\vec{v} + \vec{v}\sigma]$ of spin density σ and velocity $\vec{v}$
  - this definition has no obvious physical meaning
  - we argue that the spin-Hall current can be defined by the real-space current distribution and its spin polarization
  - both quantities can be measured (at least in principle)

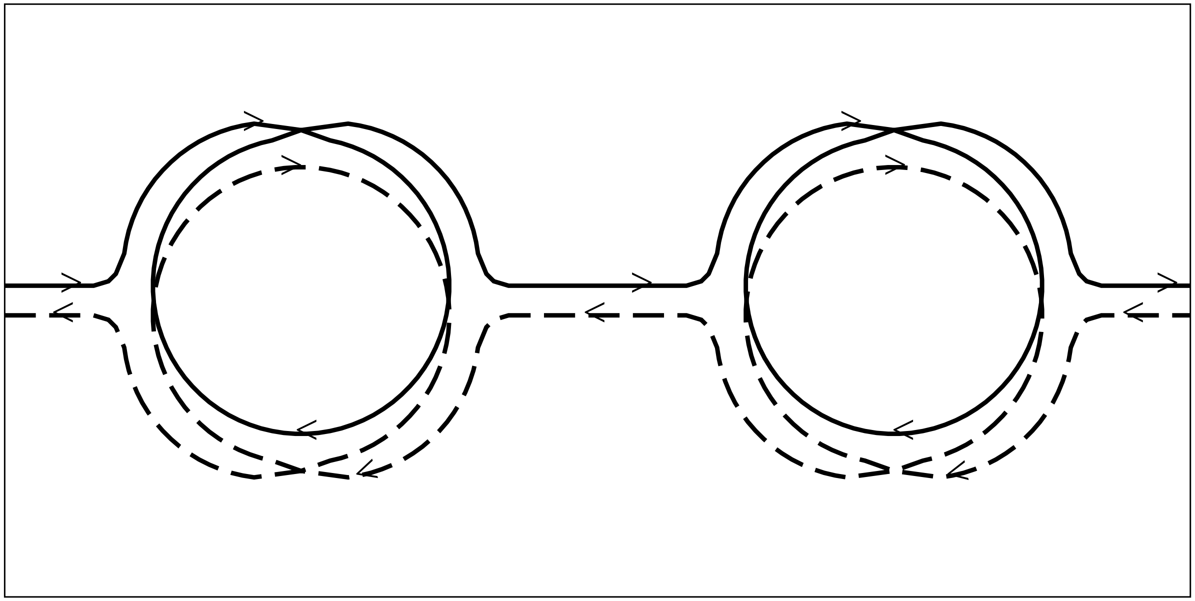
BASIC IDEA

current distribution j_x for states with k_x and $-k_x$

model: 2D cosine potential, states with $m = +1$

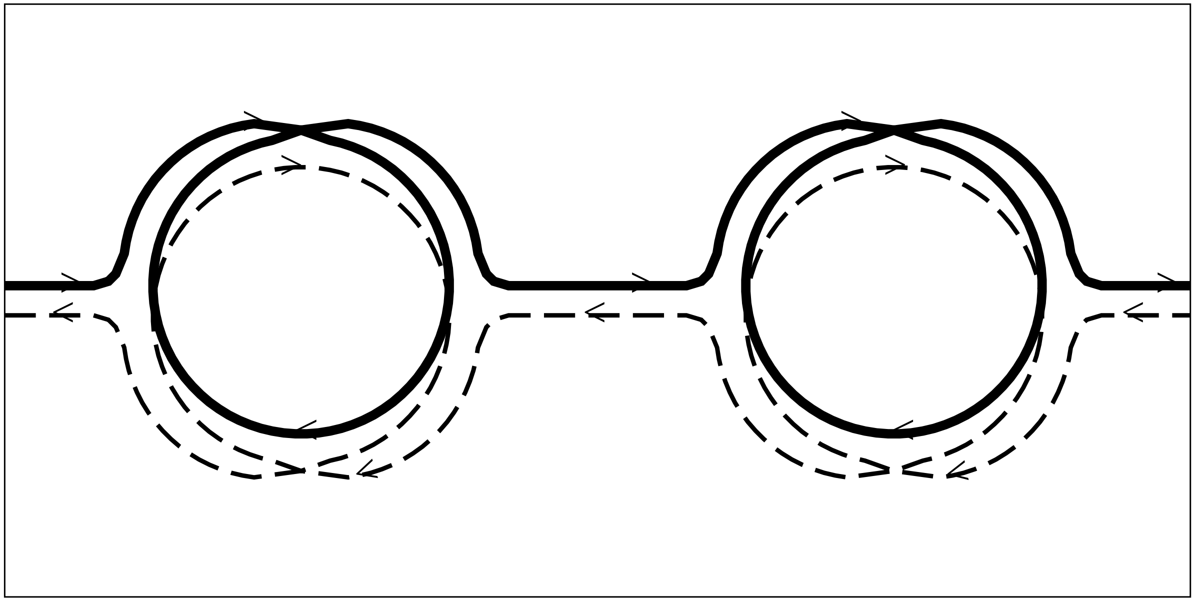


BASIC IDEA



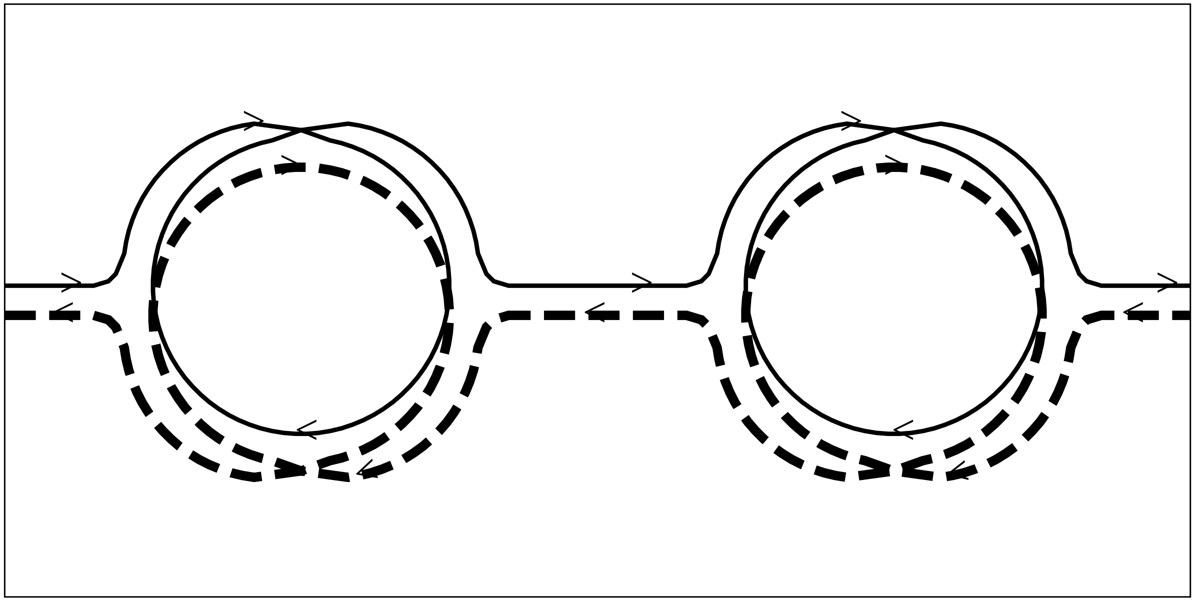
in equilibrium $\vec{j}(\vec{k}) = \vec{j}(-\vec{k})$

BASIC IDEA



out of equilibrium $\vec{j}(\vec{k}) \neq \vec{j}(-\vec{k})$

BASIC IDEA



out of equilibrium $\vec{j}(\vec{k}) \neq \vec{j}(-\vec{k})$

OUTLINE

- Formalism: empirical pseudopotential method
- Spin polarization of Bloch states
- Effective Hamiltonian for 2D electron gas
- Spin polarization of Hall current densities
- Conclusions and outlook

P. Středa, Phys. Rev. B **82**, 045115 (2010).
P. Středa and T. Jonckheere, Phys. Rev. B **82**, 113303 (2010).
P. Středa and V. Drchal, Phys. Rev. B **86**, 195204 (2012).

EMPIRICAL PSEUDOPOTENTIAL METHOD 1

$$H = H_0\sigma_0 + H_{\rm so}\,, \quad H_0 = \frac{p^2}{2m_0} + V(\vec{r})\,, \quad H_{\rm so} = \gamma\,\vec{\sigma}\cdot\left[\vec{\nabla}V(\vec{r})\times\vec{p}\right]$$

$\gamma = \frac{\hbar}{4m^2c^2} = 3.53\times 10^{-8}\,{\rm s/kg}$ ... spin-orbit coupling constant

unit matrix and Pauli matrices

$$\sigma_0 \equiv \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix},\ \sigma_x \equiv \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},\ \sigma_y \equiv \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix},\ \sigma_z \equiv \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$V(\vec{r}) = \sum_{\vec{G}}\sum_{\alpha} V_\alpha(\vec{G})e^{i\vec{G}(\vec{R}_\alpha - \vec{r})} \quad \ldots \quad \text{potential}$$

$$\langle\vec{r}|n,s,\vec{k}\rangle = \Psi_{n,s,\vec{k}}(\vec{r}) = \frac{1}{\sqrt{8\pi^3}}\,e^{i\vec{k}\vec{r}}u_{n,s}(\vec{k},\vec{r}) \quad \ldots \quad \text{Bloch functions}$$

$$u_{n,s}(\vec{k},\vec{r}+\vec{R}_i) = u_{n,s}(\vec{k},\vec{r}) \quad \ldots \quad \text{periodic part}$$

EMPIRICAL PSEUDOPOTENTIAL METHOD 2

$$u_{n,s,\vec{k}}(\vec{r}) \; = \sum_{\vec{G}} e^{i\vec{G}\vec{r}} \begin{pmatrix} C^{(1)}_{n,s,\vec{k}}(\vec{G}) \\ C^{(2)}_{n,s,\vec{k}}(\vec{G}) \end{pmatrix} \quad \ldots \quad \text{periodic part}$$

$$\vec{v}_{n,s}(\vec{k}) \; = \; \frac{1}{\hbar}\, \vec{\nabla}_{\vec{k}} E_{n,s}(\vec{k}) \quad \ldots \quad \text{velocity}$$

$$\vec{R}_{n,s}(\vec{k}) \equiv \langle n, s, \vec{k} |\, \vec{r}\, | n, s, \vec{k} \rangle \; = \; \vec{R}_{n,s}(-\vec{k}) \quad \ldots \quad \text{center of mass}$$

$$\vec{\sigma}_{n,s}(\vec{k}, \vec{r}) \equiv \Psi^{+}_{n,s,\vec{k}}(\vec{r})\, \vec{\sigma}\, \Psi_{n,s,\vec{k}}(\vec{r}) \; = \; -\,\vec{\sigma}_{n,s}(-\vec{k}, \vec{r}) \quad \ldots \quad \text{spin density}$$

M. L. Cohen and T. K. Bergstresser, Phys. Rev. **141**, 789 (1966)

K. A. Mäder and A. Zunger, Phys. Rev. **B 50**, 17393 (1994)

T. P. Humphreys and G. P. Srivastava: phys. stat. sol. (b) **112** (1982) 581

EMPIRICAL PSEUDOPOTENTIAL METHOD 3

fcc lattice

$$\mathbf{A}_1 = \frac{a}{2}(0,1,1)$$
$$\mathbf{A}_2 = \frac{a}{2}(1,0,1)$$
$$\mathbf{A}_3 = \frac{a}{2}(1,1,0)$$

2 atoms in primitive cell basis

$\boldsymbol{\tau}_1 = \frac{a}{2}(-\frac{1}{4},-\frac{1}{4},-\frac{1}{4})$ ... As
$\boldsymbol{\tau}_2 = \frac{a}{2}(\frac{1}{4},\frac{1}{4},\frac{1}{4})$ ... Ga

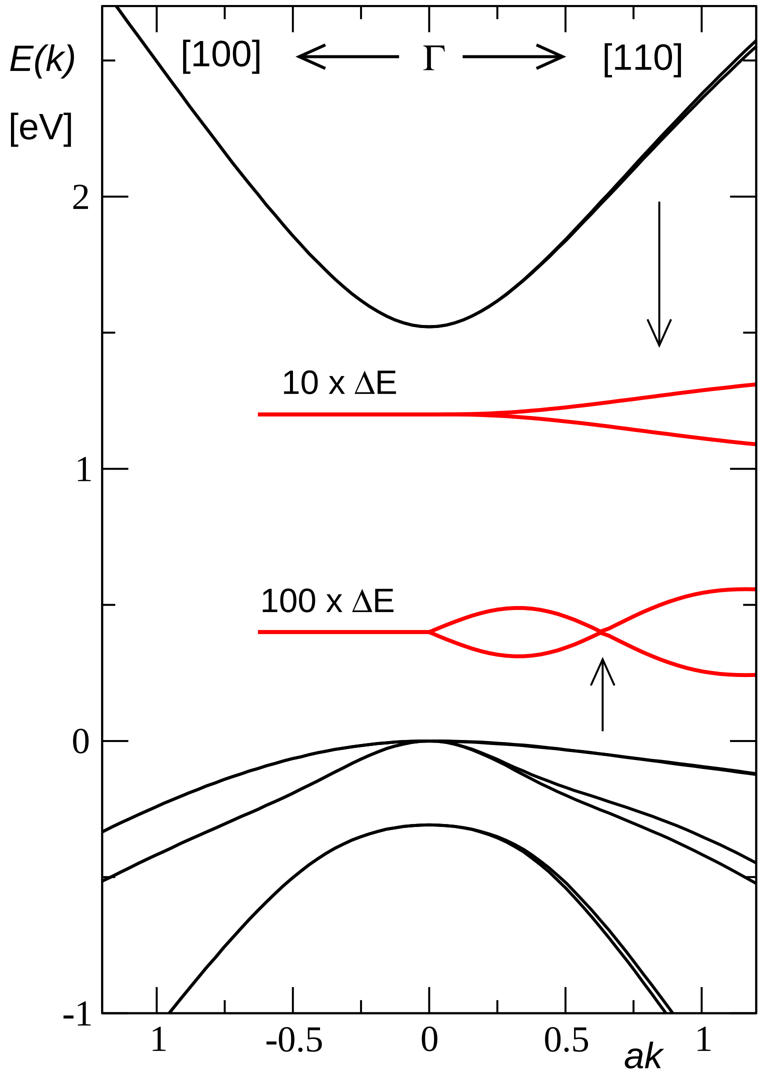
$$\boldsymbol{\tau} = \boldsymbol{\tau}_2 = -\boldsymbol{\tau}_1$$

$\frac{a}{2\pi}\mathbf{G}$	m	$v^{\mathrm{S}}(\mathbf{G})$ [Ry]	$v^{\mathrm{A}}(\mathbf{G})$ [Ry]
(111)	8	–0.23	0.07
(220)	12	0.00	0.05
(222)	8	0.01	0.00
(311)	24	0.06	0.01

Fourier components of local potential for GaAs. The quantity m denotes the multiplicity of a corresponding reciprocal lattice vector $\mathbf{G}$.

$$\begin{aligned}
\langle i\sigma|V^{\mathrm{L}}|i'\sigma'\rangle &= \delta_{\sigma,\sigma'}\left[v^{\mathrm{S}}(\mathbf{G}_{ii'})\cos(\mathbf{G}_{ii'}\cdot\boldsymbol{\tau}) + i v^{\mathrm{A}}(\mathbf{G}_{ii'})\sin(\mathbf{G}_{ii'}\cdot\boldsymbol{\tau})\right] \\
\langle i\sigma|V^{\mathrm{SO}}|i'\sigma'\rangle &= \boldsymbol{\sigma}_{\sigma\sigma'}\cdot(\mathbf{G}_i+\mathbf{k})\times(\mathbf{G}_{i'}+\mathbf{k})\,\Phi(\mathbf{G}_{ii'}) \\
\Phi(\mathbf{G}) &= -i\lambda^{\mathrm{S}}\cos(\mathbf{G}\cdot\boldsymbol{\tau}) + \lambda^{\mathrm{A}}\sin(\mathbf{G}\cdot\boldsymbol{\tau}) \\
\lambda^{\mathrm{S}} &= 0.0084\,\text{Ry}\,, \quad \lambda^{\mathrm{A}} = 0.002\,\text{Ry}
\end{aligned}$$

EMPIRICAL PSEUDOPOTENTIAL METHOD 4



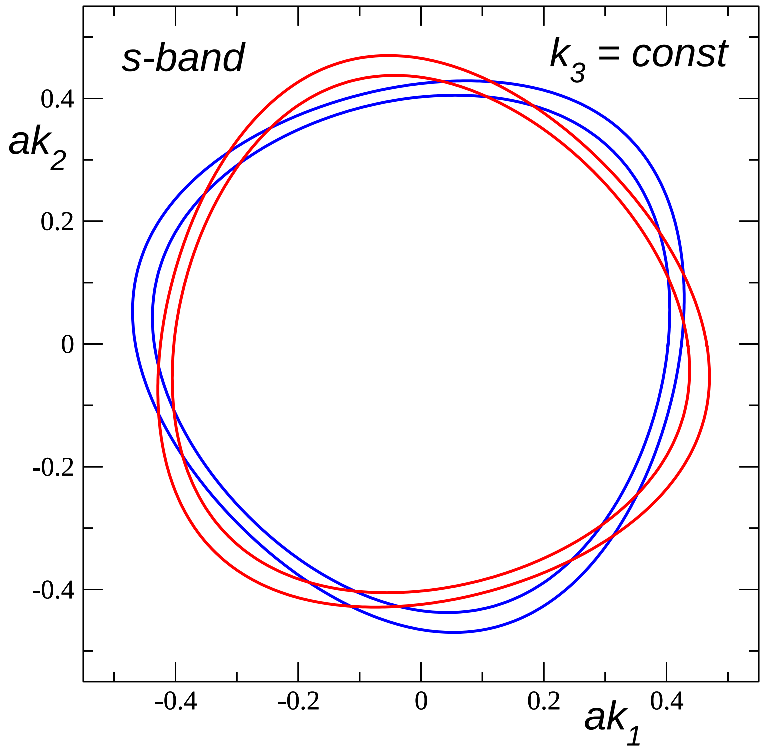
Energy dispersion laws of GaAs s- and p-bands in the vicinity of the Γ-point along the [100] and [110] directions for $k_z = 0$

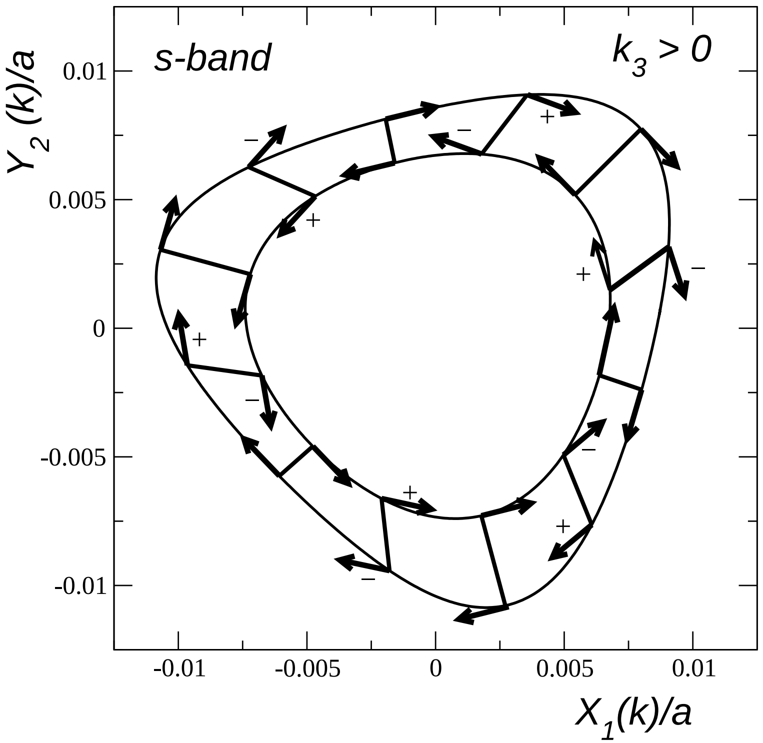
red lines: the energy difference of spin-split dispersion laws

$$\Delta E_n(\vec{k}) = E_{n,s}(\vec{k}) - E_{n,-s}(\vec{k})$$

for s-band and heavy hole p-band

SPIN POLARIZATION OF BLOCH STATES 1





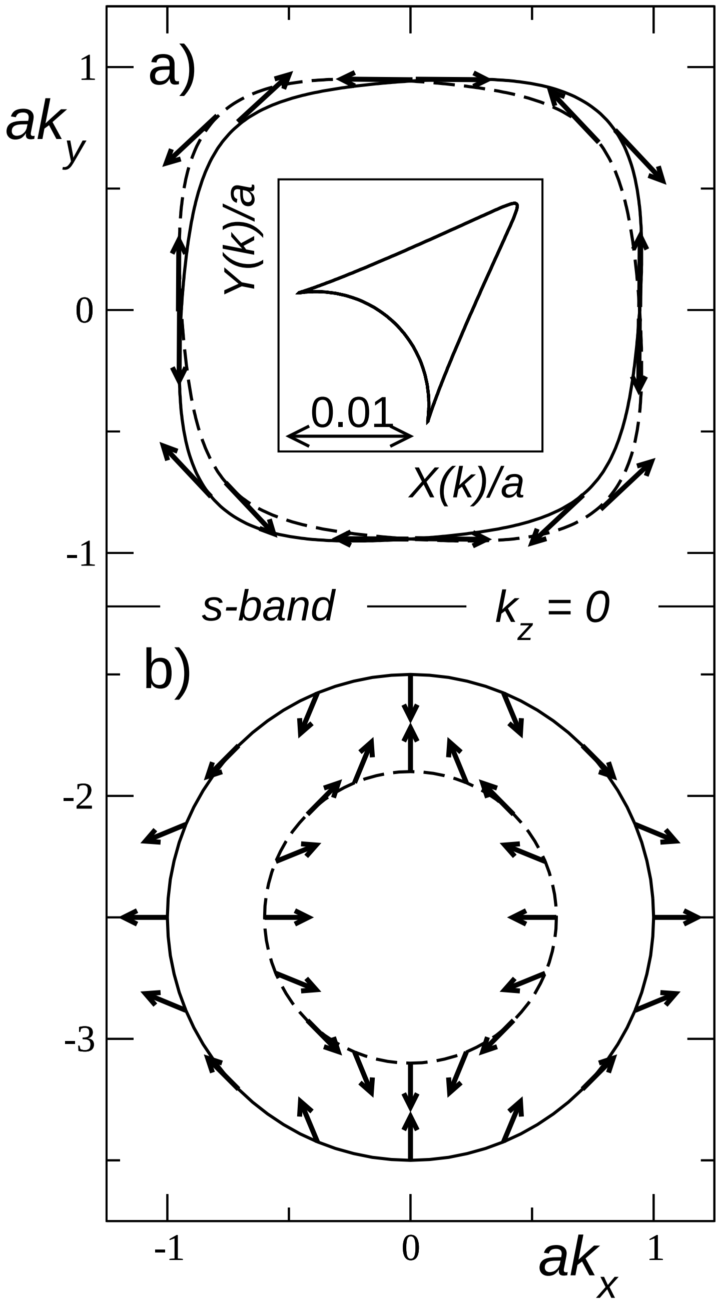
equienergy lines in the [111] plane

blue $k_3 > 0$, red $k_3 < 0$

mass-center positions

arrows: spin orientation

SPIN POLARIZATION OF BLOCH STATES 2



equienergy lines

arrows: spin orientation

inset: mass center position

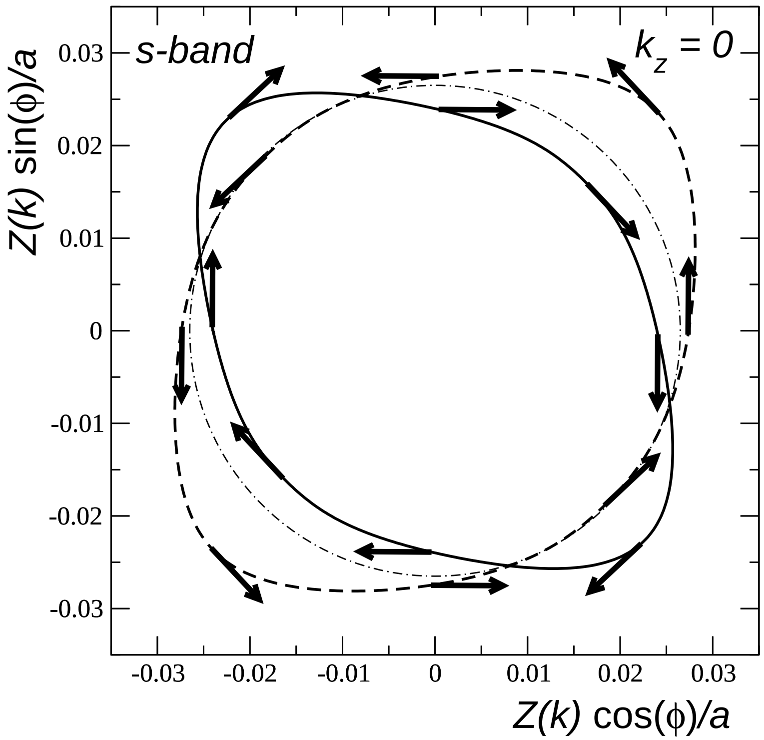
Dresselhaus-type spin orientation

arrows: spin orientation

(according to Winkler: Spin orbit coupling effects in 2D ..., Springer, 2003)

SPIN POLARIZATION OF BLOCH STATES 3

z-coordinate of mass-center positions



s-band states

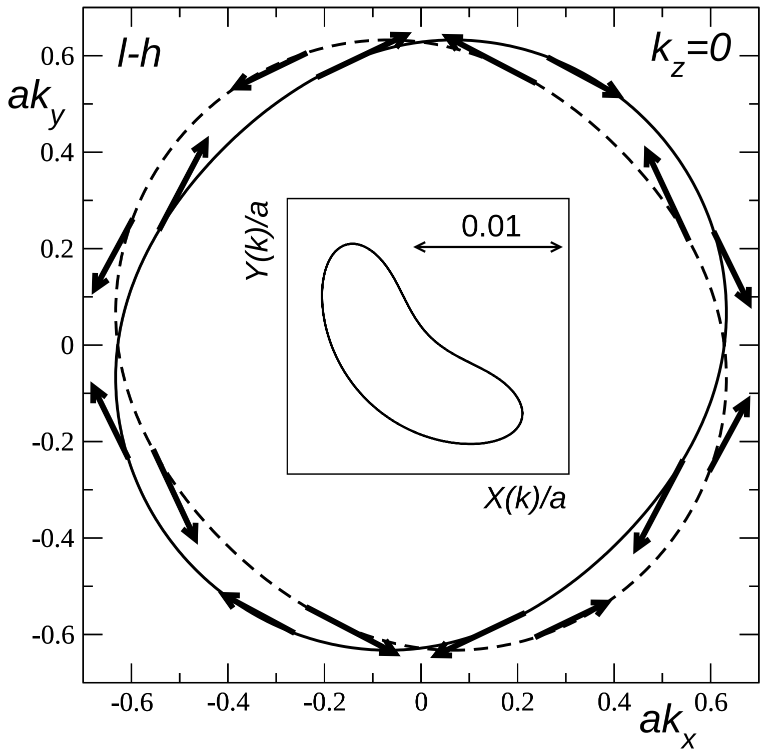
equienergy lines in [001] plane

polar graph

arrows: spin orientation

SPIN POLARIZATION OF BLOCH STATES 4

light holes



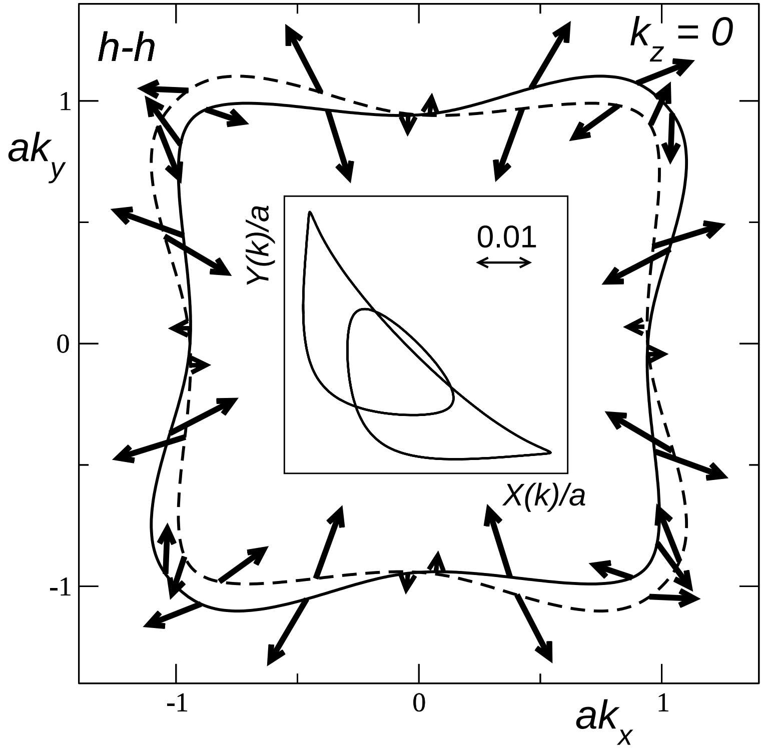
equinergy lines in [001] plane

arrows: spin orientation

inset: mass center position

SPIN POLARIZATION OF BLOCH STATES 5

heavy holes



equienergy lines in [001] plane

arrows: spin orientation

inset: mass center position

SPIN POLARIZED HALL CURRENT DENSITIES 1

$$\vec{j}_{n,s}(\vec{k},\vec{r}) \;=\; -e\,\Psi^{+}_{n,s,\vec{k}}(\vec{r})\,\vec{v}\,\Psi_{n,s,\vec{k}}(\vec{r}) \;\;\ldots\; \text{current density in state } |n,s,\vec{k}\rangle$$

$$\vec{v} \;=\; \frac{\vec{p}}{m_0}\,\sigma_0 + \gamma\,\vec{\sigma}\times\vec{\nabla}V(\vec{r}) \;\;\ldots\; \text{velocity operator}$$

electric field along the x direction induces non-equilibrium occupation of states represented by a shift Δk_x of occupied states

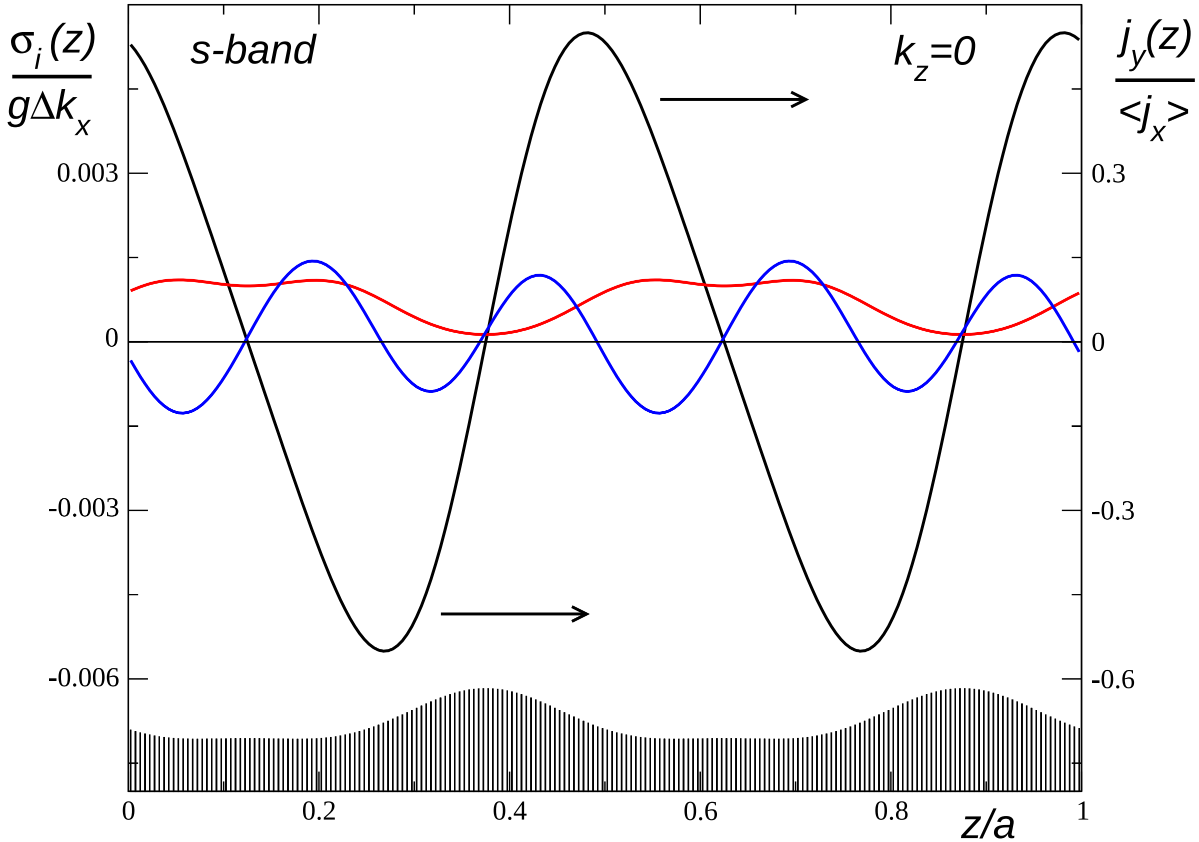
$$\frac{\vec{j}(\mu,\vec{r})}{\Delta k_x} = -\sum_{n,s}\int \delta\left(E_{n,s}(\vec{k})-\mu\right)\frac{\partial E_{n,s}(\vec{k})}{\partial k_x}\,\vec{j}_{n,s}(\vec{k},\vec{r})d\vec{k} \;\;\ldots\; \text{current density}$$

$$j_y(z) = \int \vec{j}(\mu,\vec{r})\,dx\,dy \;\;\ldots\; \text{averaged Hall current density}$$

$$\vec{\sigma}_{n,s}(\vec{k},\vec{r}) \;=\; \Psi^{+}_{n,s,\vec{k}}(\vec{r})\,\vec{\sigma}\,\Psi_{n,s,\vec{k}}(\vec{r}) \;\;\ldots\; \text{spin density in state } |n,s,\vec{k}\rangle$$

similarly as the current density above, we can define the spin density and averaged spin density

SPIN POLARIZED HALL CURRENT DENSITIES 2



Hall current density $j_y(z)$ black line

spin density $\sigma_x(z)$ red line

spin density $\sigma_y(z)$ blue line

bottom: mass density distribution $\int dxdy\,|\Psi(x,y,z)|^2$ ... function of z

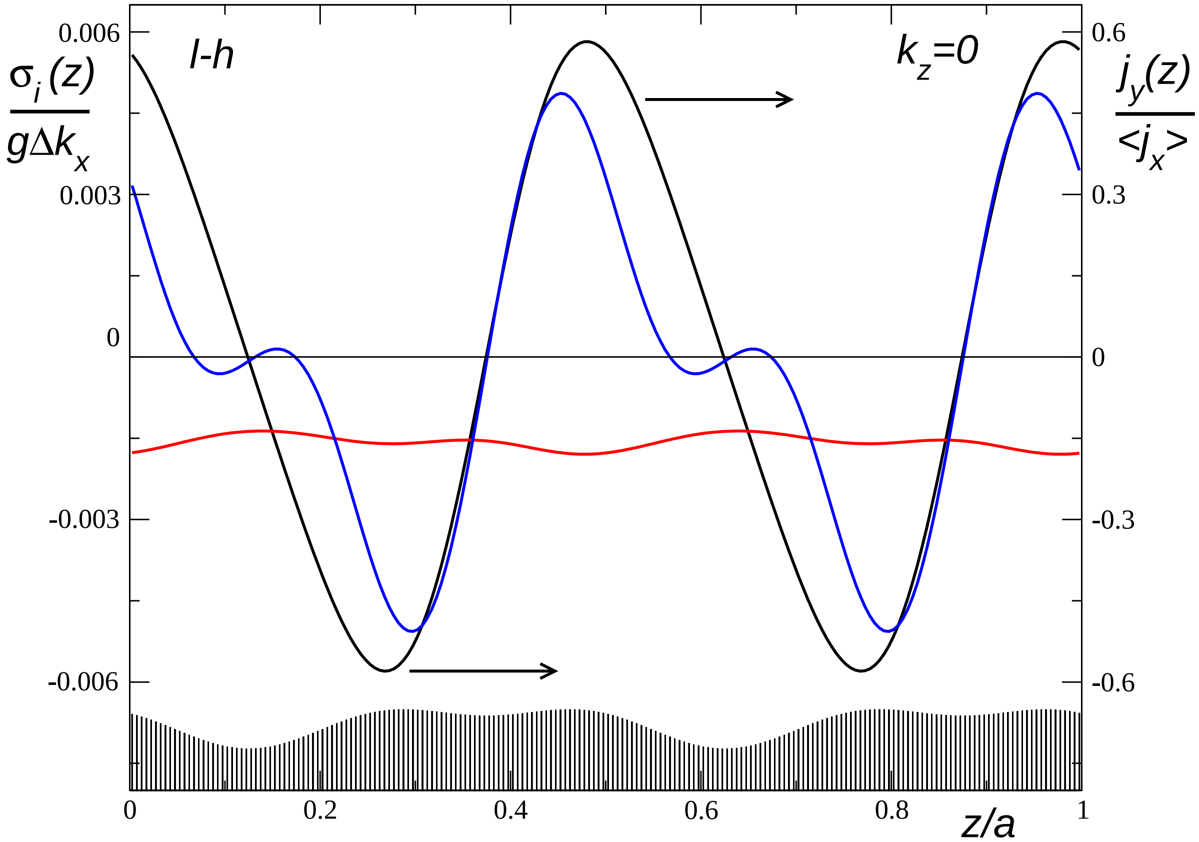
direction [001]

negligible transfer of spin

$$\int dz\, j_y(z) = \int dz\, \sigma_y(z) = 0$$

$$\int dz\, j_y(z)\sigma_y(z) \approx 0$$

SPIN POLARIZED HALL CURRENT DENSITIES 3



Hall current density $j_y(z)$ black line

transfer of spin possible

spin density $\sigma_x(z)$ red line

$$\int dz\, j_y(z) = \int dz\, \sigma_y(z) = 0$$

spin density $\sigma_y(z)$ blue line

$$\int dz\, j_y(z)\sigma_y(z) \neq 0$$

bottom: mass density distribution $\int dxdy\, |\Psi(x,y,z)|^2$ ... function of z

direction [001]

CONCLUSIONS AND OUTLOOK

- empirical pseudopotential method applied to semiconductors with zinc-blende structure
- Bloch eigenfunctions give real-space spin and current distributions
- in the current-carrying regime:
  - local spin polarization
  - spin polarized Hall current densities
  - at least light holes transfer spins of different orientation in opposite directions: this leads to spin Hall current that can be expressed via quantities that can be measured
- open problems:
  - include effects of sample edges and realistic conditions for the potential-well boundaries
  - spin accumulation at the edges gives nonzero σ_z (see T. D. Stanescu and V. Galitski, Phys. Rev. B **74**, 205331 (2006).)