Spin polarization of Bloch states and Hall currents in GaAs quantum wells

Pavel Středa$^a$ and Václav Drchal$^b$

Institute of Physics ASCR, Na Slovance 2, 182 21 Praha 8, Czech Republic

Abstract. Real-space distribution of the Hall current densities and their spin polarization in non-magnetic zinc-blende semiconductors is analysed. It is shown that the applied current gives rise to a local spin polarization accompanied by spin-polarized Hall-current densities. Especially for hole carriers they are responsible for transferring spins of different orientation in opposite directions, spin Hall current, while the total Hall current vanishes.

1 Introduction

The description of the carrier properties in zinc-blende semiconductors is usually based on the Kane or Luttinger models [1] which capture most of the semiconductor properties. A key ingredient of these models is the spin-orbit interaction which couples the momentum with the orbital and spin degrees of freedom giving rise to a spin splitting in the $k$-space. Energy spectrum and spin orientation of carriers are established by the use of the effective medium Hamiltonian [2] which depends on the wave vector $k$. In the case of the equilibrium occupation of states the total spin vanishes at any point in real space, which is the consequence of the Kramer’s theorem. However, the non-equilibrium occupation induced by the applied current leads to the spin polarization of the system [3–5]. As predicted by the spin-Hall-effect theory, [6–9] it should be accompanied by the spin-Hall current. The spin current operator is usually defined as a symmetrized product of the spin density and velocity. Unfortunately, this definition has no obvious physical meaning [10,11].

In this paper the real-space spin distribution in non-magnetic zinc-blende semiconductors will be analysed to establish the spatial distribution of the Hall current densities and their spin polarization. It will be shown that particularly for $p$-band states they are able to transfer spins of different orientation in opposite directions while the total Hall current vanishes.

Real space analysis requires the knowledge of Bloch eigenfunctions which excludes the use of the effective medium approach. We have used empirical pseudopotential method with parameters representing GaAs crystals for their evaluation [12,13]. Obtained energy dispersions as well spin polarization of Bloch states show the same features as those given by the effective medium approach.

We limit our attention to a two-dimensional carrier gas confined along the [001] crystallographic direction. Its width standardly exceeds ten lattice constants. It suggests that in this case the carrier properties could be approximated as properties of carriers in the bulk crystal with vanishing $k$-vector component perpendicular to the carrier layer, $k_z = 0$. This approximation ignoring real conditions at the potential well boundaries can thus be applicable to a two-dimensional system realized in wide enough wells.

It can be expected that the current-induced real-space distribution of the Hall current densities and their spin polarization depends on the orbital momentum of carriers. For this reason the numerical results will be presented for $s$-band electrons having nearly zero orbital momentum and light holes as an example of carriers having the $p$-type character with non-zero momentum.

2 Model Hamiltonian

Standard single-electron Hamiltonian including spin-orbit coupling is of the following form

$$H = \left[ \frac{\mathbf{p}^2}{2m_0} + V(\mathbf{r}) \right] \sigma_0 + \gamma \sigma \cdot [\nabla V(\mathbf{r}) \times \mathbf{p}] ,$$

where $\gamma$ denotes spin-orbit coupling constant $\gamma = \lambda \hbar^2 / 4 \hbar$ with Compton length $\lambda_c = \hbar / (m_0 \gamma) = 2.43 \cdot 10^{-12}$m. Components of the spin operator $\sigma$ are Pauli matrices

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

and $\sigma_0$ stands for a unit matrix. Translation symmetry of the crystalline potential $V(\mathbf{r})$ implies that eigenfunctions are of the Bloch form

$$\Psi(n, s, \mathbf{k}) = \psi_{n, \mathbf{k}, \mathbf{R}_i}(\mathbf{r}) = \frac{1}{\sqrt{V_0}} e^{i \mathbf{R}_i} u_{n, \mathbf{k}}(\mathbf{r} + \mathbf{R}_i) ,$$

where $\mathbf{R}_i$ is the position vector of the $i$-th Wigner-Seitz cell and $(n, s)$ denote energy bands. Periodic parts of Bloch functions $u_{n, \mathbf{k}}(\mathbf{r})$ are spinors which can be expressed as a Fourier series

$$u_{n, \mathbf{k}}(\mathbf{r}) = \sum_{\mathbf{G}} e^{i \mathbf{G} \cdot \mathbf{r}} \left( C^{(1)}_{n, \mathbf{k}}(\mathbf{G}) C^{(2)}_{n, \mathbf{k}}(\mathbf{G}) \right) ,$$

where $\mathbf{G}$ are reciprocal lattice vectors.
Band numbers \( n \) and \( s \) together with the wave vector \( \mathbf{k} \) define the energy dispersion law \( E_{n,s}(\mathbf{k}) \) and because of the translation symmetry the velocity expectation values are given as

\[
v_{n,s}(\mathbf{k}) = \frac{1}{\hbar} \nabla_{\mathbf{k}} E_{n,s}(\mathbf{k}).
\]

Since the spin operator does not commute with the Hamiltonian, expectation values of the spin-vector length \( |\sigma_{n,s}(\mathbf{k})| \) can generally attain any value between 0 and 1.

Crystalline potential can be generally expressed in the form of the Fourier series. Assuming that the local atomic potentials have the spherical symmetry, we get

\[
V(\mathbf{r}) = \frac{1}{\Omega_c} \sum_{\mathbf{G}} \sum_{\alpha} \Omega_{\alpha} V_{\alpha}(\mathbf{G}) e^{i\mathbf{G}\cdot\mathbf{R}_{\alpha}},
\]

where \( \mathbf{G} = |\mathbf{G}| \), index \( \alpha \) denotes the type of atom as well as its position \( \mathbf{R}_{\alpha} \) within the unit cell of the volume \( \Omega_{\alpha} \), and \( \mathbf{G} \) is the atomic volume. Instead of the real crystalline potential we consider the empirical pseudopotential \( V(\mathbf{r}) \) representing zinc-blende structure. Fourier coefficients \( V_{\alpha}(\mathbf{G}) \) representing GaAs crystals can be found in a number of publications [12,13]. Note that empirical pseudopotentials do not include the contribution of low lying core states to the spin-orbit coupling term defined in Eq.(1). To get a quantitative agreement with experimentally established energy dispersions, it is necessary to add relevant correction terms [13,14].

The eigenvalue problem for the above model gives energy bands showing general features corresponding to the zinc-blende crystal symmetry in agreement with the Dreselhaus group analysis [2]. No spin-splitting of energy bands is found along the high symmetry directions \( \Lambda \) and \( \Lambda \) defined by \( L \) and \( X \) points on the Brillouin zone boundary. Along other directions spin-splitting becomes non-zero, but it is rather weak as can be seen in Fig.1, where dispersions of \( s \)- and \( p \)-band states along [1,1,0] axis and \( \Lambda \) direction represented by [1,0,0] axis are shown.

![Fig. 1. Energy dispersion laws of GaAs s- and p-bands in the vicinity of the \( \Gamma \)-point along the [100] and [110] directions for \( k_z = 0 \). The energy difference of spin-split dispersion laws, \( \Delta E_n(\mathbf{k}) = E_{n,s}(\mathbf{k}) - E_{n,p}(\mathbf{k}) \), for s-band and heavy hole p-band are shown by dashed lines.](image1)

**3 Spin polarization of Bloch states**

Spin orientation of Bloch states strongly depends on the wave vector direction. Along the directions for which spin-splitting takes place a very rich spin structure has been found. We limit our presentation of the numerical results to states at equienergy contours in the (0,0,1) plane normal to the [0,0,1] direction having \( k_z = 0 \). In this case expectation values of \( \sigma_z \) vanishes. Since the [0,0,1] axis is a standard growth direction, these states can be considered as states representing two-dimensional systems realized in semiconductor heterostructures. For an easier presentation the equienergy contours of rather large \( k \)-radius are used since the tiny spin splitting increases approximately as \( k^2 \).

Nevertheless, the presented properties have the same qualitative features as those obtained for smaller radii of the equienergy contours.

Equienergy contours of spin-split \( s \)-band states normal to [0,0,1] crystallographic direction, 4-fold rotation axis, are shown in Fig.2 for \( k_z = 0 \) together with arrows representing spin orientation of Bloch states. No spin-splitting is observed at high symmetry axes in agreement with Dreselhaus group analysis [2]. Spin is perpendicular to the velocity direction and its length \( |\sigma(\mathbf{k})| \) approaches unity.

Equienergy contours for spin-split light-hole states normal to [001] crystallographic direction are shown in Fig.3 for \( k_z = 0 \). Spin is nearly perpendicular to the velocity direction but its length is much less than 1, \( |\sigma(\mathbf{k})| \approx 0.55 \).

Spin orientation of Bloch states of heavy-holes is rather rich as shown in Fig. 4. Spin is not perpendicular to the velocity and its length varies between 0 and 1 approaching
null
of the order as that for light holes. However, opposite to the s-state electrons and light holes the observed properties are not so universal. The reason is that their spin structure as well as the shape of equienergy lines depend on the heavy hole concentration. Note that there even appears crossing of the energy dispersions as indicated in Fig. 1 by the arrow.

Let us note that in the three-dimensional case the spin polarization becomes more complex because of the non-zero contribution of the spin z-component and non-zero Hall current densities along z-direction.

5 Concluding remarks

We have studied the spin polarization of Bloch states in semiconductors with zinc-blende structure using the empirical pseudopotential method. Knowledge of Bloch eigenfunctions allowed us to analyse real-space spin and current distributions. In the current carrying regime it results in the local spin polarization accompanied by spin-polarized Hall-current densities. We have shown that at least in the case of light holes they are responsible for transferring spins of different orientation in opposite directions. It results in the spin Hall current expressed by quantities measurable at least in principle.

Nevertheless, for full understanding of spin currents the presented analysis needs a modification allowing to take into account the effect of the sample edges together with realistic conditions for potential well boundaries. Particularly it is important in the case of the spin accumulation at the sample edges [15], which is up to now the only observable manifestation of the spin Hall effect.

References