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P Kleinert[1] and V V Bryksin[2]

[1] Paul-Drude-Institut für Festkörperelektronik, Hausvogteiplatz 5-7, 10117 Berlin, Germany
[2] Physical Technical Institute, Politekhnicheskaya 26, 194021 St Petersburg, Russia

E-mail: kl@pdi-berlin.de

Abstract
Based on a proper definition of the spin current, we investigate the spin-Hall effect of heavy holes in narrow quantum wells in the presence of Rashba spin–orbit coupling by using a spin-density matrix approach. In contrast to previous results obtained on the basis of the conventional definition of the spin current, we arrive at the conclusion that an electric-field-induced steady-state spin-Hall current does not exist in both pure and disordered infinite samples. Only an ac field can induce a spin-Hall effect in such systems. Recently, the same conclusions were derived for the Rashba model, in which the spin splitting of electron states is linear in k.

1. Introduction

The emerging field of spintronics stimulates extensive studies of the spin-Hall effect (SHE) in semiconductors with spin–orbit coupling. Recently, an intrinsic SHE, which is entirely due to spin–orbit coupling, has been predicted to appear in two-dimensional (2D) electron systems [1] and in p-doped bulk semiconductors [2].

Most theoretical studies referred to the Rashba model of a 2D electron gas, the spin–orbit coupling of which is due to the structure-inversion asymmetry of the heterostructure. For such a system, a universal intrinsic SHE was expected in a clean sample [1]. Furthermore, it was speculated that this effect is robust against impurity scattering. However, subsequent theoretical studies revealed that elastic scattering effects can lead to a complete cancellation of the total intrinsic spin-Hall current [3–7]. It was noticed that for the model of 2D electrons with k-linear Rashba spin–orbit coupling the SHE does not survive due to the scattering-induced vertex corrections. Later, it was argued that such cancellation only occurs for this very particular linear Rashba model [8]. It was pointed out that there are other generic systems, in which the intrinsic SHE is robust against disorder because vertex corrections are calculated to be zero. One example provides the k-cubic Rashba model that approximately describes the spin–orbit interaction in a 2D hole gas of a heterostructure with highly confined quantum wells. Nowadays

the old controversy about the role played by elastic scattering is replaced by a more fundamental debate about the proper definition of the spin current [9–14]. Due to non-conservation of spin, which results from spin precession, it has been argued that its definition is largely a matter of convenience [15]. In analogy to the charge current, most researchers identified the spin current simply with the expectation value of the product of spin and velocity observables. Based on this conventional definition, the spin current is expressed from a technical point of view by particular elements of the spin-density matrix, namely $f_{\lambda'}^{\lambda}(\boldsymbol{k}, \boldsymbol{\kappa} \mid t)|_{\boldsymbol{\kappa}=0}$ (with the spin quantum numbers λ, λ', the time variable t, and the quasi-momenta $\boldsymbol{k} = (\boldsymbol{k}_1 + \boldsymbol{k}_2)/2$, $\boldsymbol{\kappa} = \boldsymbol{k}_1 - \boldsymbol{k}_2$), which depend only on the quasi-momentum $\boldsymbol{k}$. These quantities are conventionally calculated from multiband Boltzmann equations. However, this procedure is not sufficiently general and even fails for particular charge transport problems. There is a subtlety related to this definition of transport coefficients. Already for the charge transport, this procedure is only justified when the interaction Hamiltonian of the system commutes with the position operator. Otherwise one has to go back to the more general definition, which expresses the charge current through the time derivative of the dipole operator [16, 17]. In this case, the current of the multiband system is not obtained from the special elements of the density matrix $f_{\lambda'}^{\lambda}(\boldsymbol{k} \mid t)$, but is calculated from quantities $\nabla_{\boldsymbol{\kappa}} f_{\lambda'}^{\lambda}(\boldsymbol{k}, \boldsymbol{\kappa} \mid t)|_{\boldsymbol{\kappa}=0}$, which requires the consideration of the $\boldsymbol{\kappa}$ dependence in kinetic equations. For charge transport, the theory of small polarons provides a famous example. In accordance with these experiences in the charge transport theory, a proper definition of the spin current has recently been put forward [11]. According to this proper definition, the spin current is expressed by the time derivative of the spin displacement. This concept of spin current has a number of remarkable advantages [11]. It is in accordance with the near-equilibrium transport theory, satisfies the Onsager relations, and provides vanishing spin currents for Anderson insulators. As a result, by determining conjugate forces, thermodynamic and electric measurements of the spin current become possible. To further illustrate the advantage of the proper definition, let us consider a particular feature of the spin current. Due to its symmetry with respect to time inversion, a finite spin current can exist even in equilibrium [9]. For simplicity we treat the Rashba model of a 2D electron gas. According to the conventional definition, there is a field-independent stationary spin-Hall current that is completely independent of the spin accumulation. In contrast, the spin-Hall current according to the proper definition turns out to be due to the initial time variation of the spin polarization and disappears in the steady state, when the spin polarization becomes constant [13].

In the present work, we study the SHE for heavy holes in III–V semiconductor quantum wells on the basis of the proper definition of the spin current by systematically deriving and solving the kinetic equations for the spin-density matrix. Recently, experimental observations of the SHE have been reported for such a system [18]. The analysis [8] of the experimental results seems to provide evidence for a close correspondence between the detected edge spin accumulation and the bulk spin currents as described by the conventional spin-Hall theory. However, this conclusion cannot be considered to be final as the spin polarization near the edges depends on the boundary conditions and may not be directly induced by spin-Hall currents far from the boundaries. The treatment of inhomogeneous and/or finite samples requires the calculation of $f_{\lambda'}^{\lambda}(\boldsymbol{k}, \boldsymbol{\kappa} \mid t)$, the $\boldsymbol{\kappa}$ dependence of which introduces a strong coupling between the spin and charge degrees of freedom even in the absence of an electric field. The theory of spin transport in finite samples has its particular own challenges.

2. Model Hamiltonian and kinetic equations

In 2D hole systems, the Rashba spin–orbit splitting of heavy hole states is due to the structure-inversion asymmetry. The one-particle Hamiltonian for heavy holes in narrow quantum wells

being subject to spin–orbit interaction of the Rashba type has the second quantized form

$$H = \sum_{k,\lambda} a_{k\lambda}^{\dagger} [\varepsilon_k - \varepsilon_F] a_{k\lambda} - \sum_{k,\lambda,\lambda'} (\hbar\vec{\omega}_k \cdot \vec{\sigma}_{\lambda\lambda'}) a_{k\lambda}^{\dagger} a_{k\lambda'}$$

$$- \mathrm{i}e\vec{E} \sum_{k,\lambda} \nabla_\kappa a_{k-\frac{\kappa}{2}\lambda}^{\dagger} a_{k+\frac{\kappa}{2}\lambda} \bigg|_{\kappa=0} + u \sum_{k,k'} \sum_{\lambda} a_{k\lambda}^{\dagger} a_{k'\lambda}, \qquad (1)$$

which is composed of creation ($a_{k\lambda}^{\dagger}$) and annihilation ($a_{k\lambda}$) operators with quasi-momentum $k = (k_x, k_y, 0)$ and spin λ. The dispersion relation of free in-plane motion is given by $\varepsilon_k = \hbar^2 k^2/2m$. Throughout, the Fermi energy ε_F is always assumed to be the largest relevant energy scale. The strength of the 'white-noise' disorder scattering is given by the scattering rate $\hbar/\tau = 2\pi u \rho_F$ with ρ_F and u denoting the 2D density of states in the absence of spin–orbit coupling and the scattering strength, respectively. For simplicity, the electric field E is oriented along the x axis. The cubic Rashba spin–orbit coupling [19–21] is obtained from the Pauli matrices and the energy

$$\hbar\vec{\omega}_k = \frac{\alpha}{2} \left[\mathrm{i}(k_+^3 - k_-^3), (k_+^3 + k_-^3), 0 \right], \qquad (2)$$

with $k_\pm = k_x \pm \mathrm{i}k_y$ and $\hbar\omega_k = \alpha k^3$. α denotes the spin–orbit coupling constant.

All information that is necessary to determine the kinetic observables is contained in the spin-density matrix, the elements of which are grouped in the following way:

$$f(k, \kappa \mid t) = \sum_{\lambda} f_{\lambda}^{\lambda}(k, \kappa \mid t), \qquad \vec{f}(k, \kappa \mid t) = \sum_{\lambda,\lambda'} f_{\lambda'}^{\lambda}(k, \kappa \mid t)\vec{\sigma}_{\lambda\lambda'}. \qquad (3)$$

Although we treat a homogeneous 2D infinite hole gas, it is indispensable to retain both the k and κ dependence of the spin-density matrix in order to calculate the proper spin current. In the thermodynamic equilibrium ($E = 0$) and to lowest order in α, the spin degree of freedom is characterized by the vector

$$\vec{f}_{\mathrm{eq}}(k \mid t) = -\hbar\vec{\omega}_k \frac{\partial n(\varepsilon_k)}{\partial \varepsilon_k}, \qquad (4)$$

with $n(\varepsilon_k)$ being twice the Fermi distribution function. With respect to the time dependence, we prefer the consideration of Laplace-transformed kinetic equations, which are derived by exploiting the Born approximation and by keeping only the lowest-order contributions of the spin–orbit interaction in the collision integral. Due to the κ dependence, the resulting kinetic equations

$$sf - \frac{\mathrm{i}\hbar}{m}(\kappa \cdot k)f + \mathrm{i}\vec{\omega}_\kappa(k) \cdot \vec{f} + \frac{e\vec{E}}{\hbar}\nabla_k f = \frac{1}{\tau}(\bar{f} - f) + n(\varepsilon_k), \qquad (5)$$

$$s\vec{f} + 2(\vec{\omega}_k \times \vec{f}) - \frac{\mathrm{i}\hbar}{m}(\kappa \cdot k)\vec{f} + \mathrm{i}\vec{\omega}_\kappa(k)f + \frac{e\vec{E}}{\hbar}\nabla_k \vec{f}$$

$$= \frac{1}{\tau}(\bar{\vec{f}} - \vec{f}) + \frac{1}{\tau}\frac{\partial}{\partial \varepsilon_k}\overline{f\hbar\vec{\omega}_k} - \frac{\hbar\vec{\omega}_k}{\tau}\frac{\partial}{\partial \varepsilon_k}\bar{f} - \hbar\vec{\omega}_k \frac{\partial n(\varepsilon_k)}{\partial \varepsilon_k}, \qquad (6)$$

are coupled to each other. An integration over the angle of the vector k is indicated by a bar over the respective quantity. In addition, we make use of the abbreviation

$$\hbar\vec{\omega}_\kappa(k) = 3\alpha \left[(k_y^2 - k_x^2)\kappa_y - 2k_x k_y \kappa_x, (k_x^2 - k_y^2)\kappa_x - 2k_x k_y \kappa_y, 0 \right]. \qquad (7)$$

The kinetic equations (5) and (6) have the same structure as their counterparts of the linear Rashba model treated in [13]. However, now both $\vec{\omega}_k$ and $\vec{\omega}_\kappa$ depend on k_x and k_y in a nonlinear manner. An analytical solution of these equations is derived in the linear response regime, when carrier heating does not play an essential role. Our calculational procedure, which is outlined in the appendix, is nothing but an iteration of these equations with respect to $\vec{E}$ and κ. Note that possible vertex corrections are automatically included in this approach.

3. Proper spin-Hall current

Based on the conventional definition, the spin-Hall current of heavy holes in III–V semiconductor quantum wells has been thoroughly treated in the literature [20]. Main results of this approach are retrieved from our kinetic equations and presented below for the sake of comparison. Our main focus refers to the proper spin current [11, 13], which is calculated from the time derivative of the spin displacement

$$\vec{j}_i(t) = \frac{3\hbar}{2} \frac{\partial}{\partial t} \sum_m \sum_{\lambda_1, \lambda_2} r_{mi} \langle a^\dagger_{m\lambda_1} a_{m\lambda_2} \rangle_t \vec{\sigma}_{\lambda_1 \lambda_2}, \tag{8}$$

where r_m is the position operator and the factor $3\hbar/2$ refers to the angular momentum of the heavy holes. Performing a Fourier transformation and an integration by parts, the Laplace transformed spin-Hall current is expressed by the equivalent equation

$$j_y^z(s) = -\mathrm{i}s \frac{3\hbar}{2} \sum_k \frac{\partial}{\partial \kappa_y} \vec{f}^z(k, \kappa \mid s) \bigg|_{\kappa=0}. \tag{9}$$

Within the linear response approach, we need only the first-order corrections of the spin-density matrix with respect to the electric field E and the quasi-momentum κ. Based on perturbation theory, analytical results for this quantity are derived in the appendix.

To start our analysis, let us first treat the field-induced spin accumulation. From the analytical solution in equation (A.4) together with (A.5) and (A.6), we conclude that there is no field-induced spin accumulation in the cubic Rashba model ($\vec{\bar{f}}_{0E} = 0$). This result should be compared with the finite current-induced spin polarization in the linear Rashba model [22]. Furthermore, in contrast to the linear Rashba model there is no spin current, which is independent of the electric field and which exists even in thermodynamic equilibrium. Both peculiarities of the cubic Rashba model are closely related to each other and are compatible with recent studies based on diffusion equations [23].

The proper spin-Hall current is calculated by inserting equation (A.9) together with (A.10) into the defining equation (9). After cumbersome but straightforward calculations, we obtain for the single non-vanishing component of the spin-Hall current

$$j_y^z(s) = -27 \frac{\alpha^2}{\hbar^2} eE\sigma \sum_k n(\varepsilon_k) k^4 \frac{\sigma^2 - 4\omega_k^2}{(\sigma^2 + 4\omega_k^2)^3}, \tag{10}$$

which indicates that all occupied states below the Fermi energy contribute. The very same feature, which is also observed in the linear Rashba model, seems to be a generic property of the intrinsic SHE [13, 21]. In equation (10), the abbreviation $\sigma = s + 1/\tau$ is used. Integrating by parts, we obtain another equivalent result, in which at zero temperature ($T = 0$) only states on the Fermi surface play a role

$$j_y^z(s) = \frac{9}{2} \frac{eE}{m} \sigma \sum_k n'(\varepsilon_k) \frac{\omega_k^2}{(\sigma^2 + 4\omega_k^2)^2}. \tag{11}$$

The time dependence of the spin-Hall current is obtained from this equation by applying an inverse Laplace transformation. The analytical result is easily obtained

$$j_y^z(t) = \frac{9}{8} \frac{eE}{m} \exp\left(-\frac{t}{\tau}\right) \sum_k n'(\varepsilon_k) (\omega_k t) \sin(\omega_k t). \tag{12}$$

From this equation, we conclude that after the electric field is switched on at time $t = 0$, $j_y^z(t)$ exhibits damped oscillations so that in the steady state, there is no spin-Hall current. At zero temperature, our main result in equation (11) takes the simple form

$$j_y^z(s) = -\frac{9}{2\pi} \frac{eE\alpha^2}{\hbar^2} \frac{\sigma k_F^6}{(\sigma^2 + 4\alpha^2 k_F^6)^2}, \tag{13}$$

where k_F denotes the Fermi momentum. From this equation, we obtain for the spin-Hall conductivity of a perfect crystal ($\tau \to \infty$) the following spin-Hall conductivity:

$$\sigma_{sH}(\omega \to 0) = \frac{9e}{8\pi\hbar^2}\left(\frac{\omega}{2\omega_{k_F}}\right)^2, \tag{14}$$

which vanishes in the limit $\omega \to 0$.

Let us now compare these results for the proper spin-Hall current with findings previously derived on the basis of the conventional definition of the spin current [20]. Applying our approach, we easily regain published results for the conventional spin-Hall current from equations (A.4) to (A.6) (concerning the relationship between the conventional definition of the spin current and the density matrix, the reader is referred to [13]). Specializing to the zero-temperature case, we obtain for the conventional spin-Hall current

$$j_y^z(s) = -\frac{9}{2\pi}\frac{eE\alpha^2}{\hbar^2 s}\frac{k_F^6}{\sigma^2 + 4\alpha^2 k_F^6}, \tag{15}$$

which leads to the universal spin-Hall conductivity

$$\sigma_{sH}(\omega \to 0) = -\frac{9e}{8\pi\hbar^2}, \tag{16}$$

for a perfect crystal ($\tau \to \infty$) in the dc limit. These results, which have previously been derived by an alternative approach [20], seem to demonstrate that the SHE is present and robust against disorder in the cubic Rashba model. However, based on the proper definition of the spin current, we obtain equations (13) and (14), from which it is concluded that the SHE is absent in an infinite heavy hole gas.

4. Summary

Recently, it has been recognized that the SHE has an intrinsic contribution due to spin–orbit interaction in a perfect crystal. This assertion has occupied a great deal of attention because of its potential for electronic devices with low power consumption. A theoretical controversy about the disorder effect that can completely eliminate the intrinsic SHE seems to be settled now: the intrinsic SHE is absent only in the simple model of a 2D electron gas with Rashba spin–orbit coupling that turns out to exhibit anomalous properties. In all other generic systems that have been specifically studied, the SHE is present and robust against disorder [8]. However, this conclusion is derived on the basis of an approach for the SHE that revealed rather unconventional properties [9–14] so that serious doubts arose on its physical relevance. A recent proper definition of the spin current [11, 13] resolves a number of difficulties of former approaches and is in line with Onsager relations that allow the application of the near-equilibrium transport theory. On the basis of this physically motivated concept of spin transport, we arrive at the conclusion that neither in the linear [13] nor in the cubic Rashba model does an intrinsic SHE exist. Only an ac electric field is able to induce a spin-Hall current. In contrast to results derived from the conventional definition of the spin current, we cannot confirm that the linear Rashba model (treated in [13]) plays an exceptional role, when the proper spin current is considered. The effect of impurities on the intrinsic SHE is crucial both for the linear and cubic Rashba model. Despite the different roles vertex corrections play in both systems, there is no proper spin-Hall current, either in the linear or in the cubic disordered Rashba model. A remarkable discrepancy between both models refers to the low-frequency dependence of the proper spin-Hall current, which is proportional to $\ln\omega$ and ω^2 for the linear and cubic Rashba model, respectively. This conclusion does not contradict recent experiments [18], which revealed edge spin accumulations. The observed spin polarization near the boundaries

certainly depends to a large extent on the boundary conditions and may not be simply due to spin Hall currents in the bulk. In an inhomogeneous system, there is always a strong coupling between the charge and spin degrees of freedom that can give rise to a number of generic effects not present in an infinite homogeneous 2D electron or hole gas. It is an interesting future task to extend the approach applicable for the bulk to the spin-transport phenomena in finite systems.

Acknowledgments

Appendix. Solution of kinetic equations

The proper definition of the spin current in equation (9) sets up our calculational scheme as a perturbational approach with respect to κ. In addition, we restrict ourselves to the linear response regime, where only the lowest-order contribution in the electric field is taken into account. Further details about the analytical solution of the kinetic equations (5) and (6) are presented in [13]. The formal solution of the kinetic equation (6) has the form

$$\vec{f} = \frac{\sigma X - 2\vec{\omega}_k \times X + 4\vec{\omega}_k(\vec{\omega}_k \cdot X)/\sigma}{\sigma^2 + 4\omega_k^2}, \tag{A.1}$$

where $\sigma = s + 1/\tau$. X comprises all angle integrated quantities as well as the κ and field contributions. This result can be used to execute the perturbational approach step by step. First, we treat the equations for $\kappa = 0$ and $E = 0$ and obtain immediately

$$f_{00} = \frac{n(\varepsilon_k)}{s} = \overline{f_{00}}, \qquad \vec{f}_{00} = -\hbar\vec{\omega}_k \frac{n'}{s}, \qquad \overline{\vec{f}_{00}} = 0, \tag{A.2}$$

where the indices 00 refer to the order in κ and E. n' is a short-hand notation for $\partial n(\varepsilon_k)/\partial\varepsilon_k$. Next, the lowest-order correction due to the electric field is calculated ($E \neq 0$, $\kappa = 0$). The kinetic equation (5) for the charge degree of freedom is easily solved

$$f_{0E} = -\frac{eE}{\sigma s}\frac{\hbar k_x}{m}n', \qquad \overline{f_{0E}} = 0. \tag{A.3}$$

Based on equation (A.1), we obtain for the spin contribution

$$\vec{f}_{0E} = \frac{\sigma R_{0E} - 2\vec{\omega}_k \times R_{0E} + 4\vec{\omega}_k(\vec{\omega}_k \cdot R_{0E})/\sigma}{\sigma^2 + 4\omega_k^2}, \tag{A.4}$$

with

$$R_{0E}^x = \alpha\frac{eE}{\hbar s}\left[n''\frac{\hbar^2 k_x k_y}{m}(k_y^2 - 3k_x^2) - 6n' k_x k_y\right], \tag{A.5}$$

$$R_{0E}^y = \alpha\frac{eE}{\hbar s}\left[n''\frac{\hbar^2 k_x^2}{m}(k_x^2 - 3k_y^2) + 3n'(k_x^2 - k_y^2)\right], \qquad R_{0E}^z = 0. \tag{A.6}$$

From this solution, we conclude that there is no field-induced spin accumulation $\overline{\vec{f}_{0E}} = 0$. This peculiarity is specific for the cubic Rashba model. Within the framework of the conventional theory, all components of the spin-density matrix that determine the spin transport have already been obtained. However, for the treatment of the proper spin current it is not sufficient to

calculate $\vec{f}(k \mid s)$; it is rather necessary to treat $\nabla_{\kappa} \vec{f}(k, \kappa \mid s)$ at $\kappa = 0$. Therefore, we have to extend the perturbational approach with respect to κ. For $\kappa \neq 0$ and $E = 0$, we obtain

$$f_{\kappa 0} = (\kappa \cdot k) \left[\frac{i\hbar n}{m\sigma s} + 3i \frac{\alpha^2 n'}{\hbar\sigma s} k^4 \right], \tag{A.7}$$

$$\vec{f}_{\kappa 0} = -\frac{i\hbar^2}{m} \frac{n'}{\sigma s} (\kappa \cdot k)\vec{\omega}_k - \frac{in}{s} \frac{\sigma\vec{\omega}_{\kappa} - 2\vec{\omega}_k \times \vec{\omega}_{\kappa} + 4\vec{\omega}_k(\vec{\omega}_k \cdot \vec{\omega}_{\kappa})/\sigma}{\sigma^2 + 4\omega_k^2}, \tag{A.8}$$

where the second term on the right-hand side of equation (A.7) can be neglected. Finally, we compute the quantity that determines the spin-Hall current in equation (9), namely the contribution, which is proportional to κ and E

$$\overline{\vec{f}_{\kappa E}^z} = \frac{\sigma \overline{\vec{R}_{\kappa E}^z} - 2\overline{(\vec{\omega}_k \times \vec{R}_{\kappa E})^z}}{\sigma^2 + 4\omega_k^2}, \tag{A.9}$$

with

$$\vec{R}_{\kappa E} = \frac{i\hbar}{m}(\kappa \cdot k)\vec{f}_{0E} - i\vec{\omega}_{\kappa}(k) f_{0E} - \frac{eE}{\hbar} \frac{\partial}{\partial k_x} \vec{f}_{\kappa 0} + \frac{1}{\tau} \frac{\partial}{\partial \varepsilon_k} \overline{\hbar\vec{\omega}_k f_{\kappa E}}. \tag{A.10}$$

After a lengthy but straightforward calculation, we obtain the result for the spin-Hall current in equation (10) from (A.9), (A.10), and (9).

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