Spin-Hall transport of heavy holes in III-V semiconductor quantum wells

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We investigate spin transport of heavy holes in III-V semiconductor quantum wells in the presence of spin-orbit coupling of the Rashba type due to structure-inversion asymmetry. Similarly to the case of electrons, the longitudinal spin conductivity vanishes, whereas the off-diagonal elements of the spin-conductivity tensor are finite giving rise to an intrinsic spin-Hall effect. For a clean system we find a closed expression for the spin-Hall conductivity depending on the length scale of the Rashba coupling and the hole density. In this limit the spin-Hall conductivity is enhanced compared to its value for electron systems, and it vanishes with increasing strength of the impurity scattering. As an aside, we also derive explicit expressions for the Fermi momenta and the densities of holes in the different dispersion branches as a function of the spin-orbit coupling parameter and the total hole density. These results are of relevance for the interpretation of possible Shubnikov–de Haas measurements detecting the Rashba spin splitting.

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I. INTRODUCTION

In the last years, the emerging field of spin electronics has become a major branch of solid state physics and comprises by now all kinds of spin-dependent phenomena in semiconductor structures and related systems.1–3 Most recently, the possibility of spin-Hall currents has attracted considerable theoretical interest.4–19 In these studies a spin current (as opposed to a charge current) driven by an electric field perpendicular to it was investigated, where the spinful itinerant charge carriers are bulk valence-band holes in III-V zinc blende semiconductors4–9 or conduction band electrons in quantum wells10–19 of the same type of materials. In the present work we extend these studies to the case of heavy holes in quantum wells being subject to spin-orbit coupling of the Rashba type due to structure-inversion asymmetry.20–24

From a historical perspective, the notion of the spin-Hall effect in systems of itinerant spinful charge carriers was considered first by Dyakonov and Perel25 in the early 1970’s, and in a more recent paper by Hirsch.26 In these studies the predicted spin-Hall effect is due to spin-orbit effects influencing scattering processes upon static impurities. Following the terminology used in Refs. 10 and 5 this is referred to as the extrinsic spin-Hall effect since it necessarily requires spin-dependent impurity scattering. This is in contrast to the intrinsic spin-Hall effect studied theoretically very recently in Refs. 4–19, which is entirely due to spin-orbit coupling terms in the single-particle carrier Hamiltonian and occurs even in the absence of any scattering process. We note that this distinction between intrinsic and extrinsic effects becomes ambiguous in the limit of weak spin-orbit coupling when life time effects of carrier quasiparticles have to be taken into account.11

Yet another type of spin-Hall effect was studied recently by Meier and Loss27 in a two-dimensional Heisenberg model consisting of nonitinerant spins, in contrast to the itinerant-carrier systems mentioned before. In the case of conduction-band electrons in III-V semiconductor quantum wells, the intrinsic spin-Hall effect results from spin-orbit coupling of the Rashba type (due to structure-inversion asymmetry28) and/or the Dresselhaus type (due to bulk-inversion asymmetry29). Moreover, the interplay of these two effects leads to particularly interesting transport effects.30,31,12 For bulk valence band holes the effects of spin orbit coupling underlying the intrinsic spin-Hall effect are incorporated in Luttinger’s effective Hamiltonian32 giving rise to two different dispersion branches differing in their effective masses and known as heavy and light holes. Within this description, these states form for a given wave vector multiplets of total angular momentum 3/2 resulting from the s=1/2 spin degree of freedom of the holes and the ℓ=1 orbital angular momentum of the p-type atomic orbitals forming the valence band.33 In a quantum well, a splitting between the heavy and light holes occurs due to the size quantization in the growth direction of the heterostructure. For a sufficiently narrow quantum well and for not too high densities and temperatures, only the lowest heavy hole subbands are significantly occupied. Here the angular momentum of the heavy hole states points predominantly along the growth direction,24 corresponding to the total angular momentum states ±3/2, an approximation we shall adopt in the present work.

Experimental investigations of such systems include studies of spin polarization and transitions to an insulating state induced by magnetic fields.34 Moreover, the spin splitting due to spin-orbit coupling has been studied in detail via Shubnikov–de Haas oscillations35,36 including also anisotropic properties of the magnetoresistance.37 In recent theoretical investigations the anisotropies in the effective g factor,38 spin polarizations,39 and controlled spin rotations induced by Rashba-type spin-orbit coupling in a spin-FET setup33 have been considered. In the present work we investigate the spin-Hall effect for heavy holes in III-V zinc blende semiconductor quantum wells.

This paper is organized as follows. In Sec. II we discuss the Rashba model for heavy holes in III-V semiconductor quantum wells. As an aside, we also give explicit expressions for the Fermi momenta and the densities of holes in the different dispersion branches as a function of the spin-orbit coupling parameter and the total hole density. Apart from the present investigations, we expect these results to be also of
relevance for the interpretation of possible Shubnikov–de Haas measurements\textsuperscript{40,41} in such hole systems. Section III is devoted to the discussion of our results on spin-Hall transport, and we close with conclusions in Sec. IV.

II. RASHBA SPIN-ORBIT COUPLING FOR HEAVY HOLES

We consider the following single-particle Hamiltonian incorporating spin-orbit coupling due to structure-inversion asymmetry for heavy holes in III-V semiconductor quantum wells of appropriate growth geometry\textsuperscript{20-24}

\[ \mathcal{H} = \frac{\hat{p}^2}{2m} + \frac{i\alpha}{2\hbar^3}(p^3\sigma_+ - p^3\sigma_-), \]  

(1)

using the notations \( p_\pm = p_x \pm ip_y, \) \( \sigma_\pm = \sigma_x \pm i\sigma_y, \) where \( \hat{p}, \hat{\sigma} \) denote the hole momentum operator and Pauli matrices, respectively. These Pauli matrices operate on the total angular momentum states with spin projection \( \pm 3/2 \) along the growth direction; in this sense they represent a pseudospin degree of freedom rather than a genuine spin \( 1/2. \) In the above equation, \( m \) is the heavy-hole mass, and \( \alpha \) is Rashba spin-orbit coupling coefficient due to structure inversion asymmetry across the quantum well grown along the [001] direction chosen as the \( z \) axis. For a symmetrically grown quantum well, the coefficient \( \alpha \) is essentially proportional to an electric field applied across the well and therefore experimentally tunable\textsuperscript{20-22} This Hamiltonian has two dispersion branches given by

\[ e_s(k) = \frac{\hbar^2k^2}{2m} \pm \alpha k^3 \]  

(2)

with eigenfunctions

\[ \langle \hat{\mathbf{r}} | k, \pm \rangle = \frac{e^{ik\cdot\hat{\mathbf{r}}}}{A\sqrt{2}} \left( \frac{1}{\sqrt{\pi}} \Theta(k_y + ik_x)^2/k^3 \right), \]  

(3)

where \( \hat{\mathbf{r}} \) is the hole lattice momentum and \( A \) is the area of the system. We note that the validity of above model given by the Hamiltonian (1) is restricted to sufficiently small wave numbers and densities. In fact, the lower of the two dispersion branches (2) is (for \( \alpha > 0 \)) not bounded from below for large wave numbers and has non-negative eigenenergies only for \( k = \hbar^2/2m\alpha \) with a maximum at \( k = \hbar^2/3m\alpha. \) The unbounded decrease of the single-particle energies with increasing wave number for \( k > \hbar^2/3m\alpha \) is clearly an unphysical feature of the model. Therefore, the following considerations are restricted to sufficiently small densities such that (at zero temperature) only states with wave numbers \( k \leq \hbar^2/3m\alpha \) are occupied.

For a given Fermi energy \( \varepsilon_f \) and vanishing temperature, the above two dispersion branches give rise to two different Fermi wave numbers \( k^\pm_f \) fulfilling

\[ \varepsilon_f = \frac{\hbar^2(k^\pm_f)^2}{2m} \pm \alpha(k^\pm_f)^3 \]  

(4)

with \( k^+_f < k^-_f \) \( (k^+_f > k^-_f) \) for positive (negative) \( \alpha. \) Subtracting these two equations one finds

\[ 0 = \frac{\hbar^2}{2m}[(k^+_f)^2 - (k^-_f)^2] + \alpha[(k^+_f)^3 + (k^-_f)^3] \]  

(5)

or, cancelling a factor of \( (k^+_f+k^-_f),\)

\[ k^+_f k^-_f = -\frac{\hbar^2}{2m\alpha}((k^+_f - k^-_f) - (k^+_f + k^-_f)^2). \]  

(6)

Note that in the relations (5) and (6) the Fermi energy does not enter explicitly. In fact, the quantity which can be immediately controlled experimentally is not the Fermi energy but the hole density \( n \) given by

\[ n = \frac{1}{4\pi}[(k^+_f)^2 + (k^-_f)^2]. \]  

(7)

Combining Eqs. (6) and (7), one obtains

\[ k^+_f - k^-_f = -\frac{\hbar^2}{2m\alpha} \left[ 1 - \sqrt{1 - \left( \frac{2m\alpha}{\hbar^2} \right)^2/4\pi n} \right]. \]  

(8)

\[ k^+_f k^-_f = 4\pi n - \left( \frac{\hbar^2}{2m\alpha} \right)^2 \left[ 1 - \sqrt{1 - \left( \frac{2m\alpha}{\hbar^2} \right)^2/4\pi n} \right]. \]  

(9)

Note that for \( k^+_f \leq \hbar^2/3m\alpha \) the radicand in the above equations is always positive. Using

\[ 4\pi n = (k^+_f + k^-_f)^2 - 2k^+_f k^-_f \]  

(10)

one derives from the above equations the following explicit expression for \( k^+_f \) as a function of the density \( n \) and the Rashba parameter \( \alpha: \)

\[ k^+_f = \frac{1}{2m\alpha} \left[ \frac{\hbar^2}{2m\alpha} \left[ 1 - \sqrt{1 - \left( \frac{2m\alpha}{\hbar^2} \right)^2/4\pi n} \right] \right] + \left\{ -\frac{1}{2} \left( \frac{\hbar^2}{2m\alpha} \right)^2 \left[ 1 - \sqrt{1 - \left( \frac{2m\alpha}{\hbar^2} \right)^2/4\pi n} \right] \right\} + 3\pi n \right\} \}

(11)

The difference \( \Delta n \) of densities of holes in the two dispersion branches

\[ \Delta n = \frac{1}{4\pi}[(k^+_f)^2 - (k^-_f)^2], \]  

(12)

can be expressed as

\[ \Delta n = -\frac{1}{4\pi m\alpha} \left[ 1 - \sqrt{1 - \left( \frac{2m\alpha}{\hbar^2} \right)^2/4\pi n} \right] \times \left\{ -2 \left( \frac{\hbar^2}{2m\alpha} \right)^2 \left[ 1 - \sqrt{1 - \left( \frac{2m\alpha}{\hbar^2} \right)^2/4\pi n} \right] + 12\pi n \right\} \}

(13)

Such a difference in densities in the two dispersion branches could be experimentally detected in Shubnikov–de Haas measurements, as it was shown earlier for the case of electrons.\textsuperscript{40,41} We note that the above results for the Fermi momenta and \( \Delta n \) depend only on the total hole density \( n \) and length scale \( m\alpha/\hbar^2 \) given by the Rashba coupling.\textsuperscript{42} Winkler \textit{et al.}\textsuperscript{22} have studied both theoretically and experimentally
the magnitude of the Rashba spin orbit coupling in GaAs-based quantum well samples with heavy-hole densities of a few $10^{14}$ m$^{-2}$ and have found typical values for the characteristic length $ma^2/h^2$ of a few nanometers. In Fig. 1 we have plotted the Fermi wave numbers $k^+_f$ and the difference $\Delta n$ of holes in the two dispersion branches as a function of $ma^2/h^2$ at a total hole density of $n=3 \times 10^{14}$ m$^{-2}$.

On the other hand, solving Eq. (8) for $\alpha$ gives a convenient expression for the Rashba coefficient as a function of the total hole density and the difference of the Fermi wave numbers

$$\alpha = \frac{\hbar^2}{2m} \frac{2(k^+_f + k^-_f)}{(k^+_f - k^-_f)^2 + 4\pi n}. \quad (14)$$

Finally, writing Eq. (4) in the form

$$\epsilon_f = \frac{\hbar^2}{2m k^+_f} \pm \alpha \quad (15)$$

one obtains by adding these two equations

$$\frac{2m}{\hbar^2} \epsilon_f = \frac{1}{k^+_f} \left[ \frac{1}{k^+_f} - \frac{1}{k^+_f} \right] + \frac{1}{k^-_f} k^-_f = 1, \quad (16)$$

which does not explicitly depend on the Rashba parameter $\alpha$. From this relation, it follows with the help of Eq. (6)

$$\epsilon_f = \frac{\alpha (k^+_f k^-_f)^2}{k^+_f - k^-_f}. \quad (17)$$

Using Eqs. (8) and (9) it is straightforward to obtain from this expression an explicit relation between the Fermi energy $\epsilon_f$ and the hole density $n$ at a given Rashba parameter $\alpha$.

III. SPIN-HALL TRANSPORT

We now investigate the possibility of spin-Hall transport of heavy holes in III-V semiconductor quantum wells in the presence of Rashba-type spin-orbit coupling. We are interested in spin currents (as opposed to charge currents) as the linear response of the system to an electric field applied in the plane of the well. As we shall see below, in such a system the spin current is always perpendicular to the driving electric field and therefore Hall type. We concentrate on the case of zero temperature.

The single-particle spin current operator is defined by

$$j^{Sz}_z = \frac{3\hbar}{2} \left( \sigma^x \bar{\nu} + \bar{\nu} \sigma^x \right) = \frac{3\hbar}{2} \frac{\bar{\nu}}{m} \sigma^x, \quad (18)$$

where the factor of $3/2$ reflects the angular momentum number of the heavy holes. The hole velocity operator reads $\bar{\nu} = [\mathcal{H}, \mathcal{F}]/\hbar$ with $\mathcal{F}$ being the position operator or, in terms of components,

$$v_x = \frac{p_x}{m} + \frac{\alpha}{\hbar} \left[ 6p_y p_x \sigma^z + 3(p^2_x - p^2_y) \sigma^x \right], \quad (19)$$

$$v_y = \frac{p_y}{m} + \frac{\alpha}{\hbar} \left[ 3(p^2_x - p^2_y) \sigma^x + 6p_y p_x \sigma^y \right]. \quad (20)$$

A rigorous expression for the spin conductivity, i.e., the linear transport coefficient for spin currents driven by a spatially homogeneous in-plane electric field, is given by the Kubo formula with full frequency dependence for an electric field

$$\sigma_{xx}^{Sz}(\omega) = \frac{e}{2\pi} \sum_{\vec{k},\mu} \int_{-\infty}^{\infty} e^{i(\omega + i\eta)\tau} f[\epsilon_\mu(\vec{k})] \times \langle \vec{k}, \mu | j^{Sz}_z(t), v_x(0) \rangle | \vec{k}, \mu \rangle, \quad (21)$$

where we have concentrated on the off-diagonal $xy$ components. Moreover, we have assumed zero temperature $T=0$ and noninteracting carriers, which allows us to formulate the two-body Green’s function entering the conductivity Kubo formula in terms of single-particle operators. $e = |e|$ is the elementary charge and $f[\epsilon_\mu(\vec{k})]$ is the $T=0$ Fermi distribution function for energy $\epsilon_\mu(\vec{k})$ at wave vector $\vec{k}$ in the dispersion branch $\mu \in \{+, -, \}$. The spin-current operator (in the Dirac picture) for spin moment polarized along the $z$ direction and flowing in the $x$ direction is given by

$$j^{Sz}_x(\tau) = e^{i\tau \hbar / 2} j^{Sz}_x(0) e^{-i\tau \hbar / 2} = \frac{3\hbar}{2m} \sigma^z(t) p_x(t). \quad (22)$$

From now on we will assume the Hamiltonian generating the above time evolution to include also scattering potentials from static random impurities being present in the quantum well. The right-hand side of Eq. (21) is to be understood in the limit of vanishing imaginary part $\eta \to 0$ in the frequency argument. This imaginary part in the frequency reflects the fact that the external electric field is assumed to be switched on adiabatically starting from the infinite past of the system, and it also ensures causality properties of the retarded Green’s function occurring in Eq. (21). In general the limiting process $\eta \to 0$ does not commute with other limits and, in particular, the dc limit $\omega \to 0$ has to be taken with care. In the presence of random impurity scattering, the retarded two-body Green’s function in Eq. (21) will generically have a
frequency argument with positive imaginary part. In this
case the limit \( \eta \rightarrow 0 \) is unproblematic, and the imaginary part
of the frequency argument is just due to impurity scattering
and/or other (many-body) effects. For the present problem of
impurity scattering of noninteracting carriers being subject to
Rashba-type spin-orbit coupling, the resulting imaginary part
\( \eta > 0 \) in the frequency argument is given, to lowest order in
the Rashba coefficient and the impurity potential, by the in-
verse of the momentum relaxation time. This is certainly a
very intuitive result; the formal arguments leading to it is
completely analogous to the ones used in Ref. 11 and can be
given along the following lines: In lowest order in the spin-
orbit coupling and the impurity scattering the time-dependent
spin-current operator reads

\[ j_x^s(t) = \frac{3h}{2m} \sigma_0(t) p^0_x(t), \tag{23} \]

where the time evolution of \( \sigma_0 \) is only due to the Hamil-
tonian (1), while \( p^0_x(t) \) contains the impurity scattering but
not the spin-orbit coupling. Now it is useful to note that, in
order to compute the expectation values in the Kubo formula
Eq. (21), only matrix elements of the time-dependent momen-
tum operator \( p^0_x(t) \) which are diagonal in the wave vector
index are needed. This enables to apply superoperator tech-
niques developed in Refs. 44 yielding

\[ [p^0_x(t)]_{k \xi} = [e^{-iH0} p^0_0(0)]_{k \xi} = [e^{-i\tau\sigma_0} p^0_0(0)]_{k \xi}, \tag{24} \]

where \( \Omega_0 \) is the scattering master operator in lowest order of
the scattering potential. This operator is the same as it oc-
curs as the scattering term in the usual Boltzmann equation
when evaluated in lowest order via Fermi’s golden rule. Thus,
Eq. (24) describes the usual momentum relaxation due to
static impurities in lowest order in the scattering potential.
For impurity potentials being isotropic in real space, the
momentum \( p^0_x \) is an exact eigenfunction of \( \Omega_0 \), and the eigen-
value is given by the well-known inverse momentum relaxation
time \( 1/\tau(\varepsilon) \) (Refs. 44 and 45) which in general depends
on the energy \( \varepsilon(\tilde{k}) \). To lowest order in the Rashba coupling,
this energy argument can be replaced with the Fermi energy
in the absence of spin-orbit interaction. We note that this
momentum relaxation rate \( 1/\tau \) is the same as obtained in the
standard diagrammatic approach and thus contains the vertex
correction for particle transport. However, this vertex cor-
rection vanishes for short-range isotropic scatterers.

The question of vertex corrections to the spin-Hall trans-
port was also examined very recently by Inoue, Bauer, and
Molenkamp, and by Dimitrova for the case of electrons be-
ing subject to Rashba spin-orbit interaction. There the au-
thors reach the conclusion that for small but finite disorder
the spin-Hall conductivity should identically vanish due to
vertex corrections, while it has its “universal value” of \( e/18\pi \)
in the case of a perfectly clean system. However, Murakami
has studied vertex correction to spin-Hall trans-
port of holes in bulk \( \text{p-type} \) semiconductors described by a
Luttinger Hamiltonian. There the author concludes that ver-
tex correction vanish identically, validating, the results of
Ref. 31, and ascribes this observation to the fact that the
underlying Hamiltonian is invariant under inversion of mo-
menta, in contrast to the Rashba Hamiltonian. These tech-
nically rather involved issues are to the opinion of the present
authors not entirely settled yet and presently under inves-
tigation.

Let us now turn to the evaluation of the spin-Hall conduc-
tivity using the aforementioned approximations. A straight-
forward calculation yields

\[ \sigma_{xy}^S(\omega) = -\sigma_{yx}^S(\omega) = -\frac{e^2}{\pi^2} \int_{k_f} \frac{k^2}{\omega^2 + \frac{i}{\tau}}\left(\frac{2ao^3}{h}\right)^2, \tag{25} \]

where, according to the above arguments, the imaginary part
of the frequency argument is given by the momentum relax-
tion rate \( 1/\tau \). Moreover, the longitudinal spin conductivities
\( \sigma_{xx}^S, \sigma_{yy}^S \) turn out of be identically zero. This is similar to the
case of electrons in a quantum well being subject to spin-
orbit coupling of either the Rashba or the Dresselhaus
type. There a longitudinal spin conductivity occurs only
if both the Rashba and the Dresselhaus coupling are present.

The remaining integral in the above expression (25) is el-
mentary; however, it leads to a rather cumbersome expres-

\[ \sigma_{xy}^S(\omega) = -\sigma_{yx}^S(\omega) = -\frac{e^2}{\pi^2} \int_{k_f} \frac{k^2}{\omega^2 + \frac{i}{\tau}}\left(\frac{2ao^3}{h}\right)^2, \tag{26} \]

where the Fermi wave numbers are given by Eq. (11). In the
opposite case \( \varepsilon_R \ll \hbar/\tau \), the leading contribution to the spin-
Hall conductivity reads

\[ \sigma_{xy}^S(\omega) = -\sigma_{yx}^S(\omega) = -\frac{e^2}{\pi^2} \int_{k_f} \frac{k^2}{\omega^2 + \frac{i}{\tau}}\left(\frac{2ao^3}{h}\right)^2, \tag{27} \]

Note that this result for the spin-Hall conductivity depends
only on the length scale \( ma/\hbar^2 \) of the Rashba coupling and the
total hole density \( n \), but not separately on quantities such as
the Fermi energy and the effective heavy hole mass. If \( ma/\hbar^2 \)
is small against the inverse square root of the total
hole density (but still fulfilling \( \varepsilon_R \ll \hbar/\tau \)), the spin-Hall con-
ductivity approaches a value of \( \sigma_{xy}^S \sim 9e/8\pi \). This is the case
if \( \hbar/\tau \ll \varepsilon_R \ll \varepsilon_p \) since \( \varepsilon_p \) is the Fermi energy. This above value
should be compared with the universal value of \( e/18\pi \) found for the spin-Hall conduc-
tivity of electrons being subject to a Rashba coupling domin-
ating possible impurity scattering. In this limit, the hole
spin-Hall conductivity is enhanced compared to the case of
electrons by a factor of \( 9 \), which is partially due to
the larger angular momentum of the heavy holes. In Fig. 2 we
have plotted the spin-Hall conductivity for dominating
Rashba coupling \( \varepsilon_R \ll \hbar/\tau \), see Eq. (27) as a function of
\( ma/\hbar^2 \) at a total hole density of \( n = 3 \times 10^{14} \text{ m}^{-2} \). As seen

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spin conductivity vanishes, whereas the off-diagonal elements of the spin-conductivity tensor are finite giving rise to an intrinsic spin-Hall effect. For a clean system we find a closed expression for the spin-Hall conductivity depending on the length scale of the Rashba coupling and the hole density. In this limit the spin-Hall conductivity is enhanced compared to its value for electron systems. For dirtier $p$-doped quantum wells when the impurity scattering dominates the spin-orbit coupling, the spin-Hall conductivity naturally vanishes as also found previously for the case of electrons. As an aside, we give explicit expressions for the Fermi momenta and the densities of holes in the different dispersion branches as a function of the spin-orbit coupling parameter and the total hole density. These results are expected to be helpful for the interpretation of possible Shubnikov–de Haas experiments aiming at the detection of the Rashba spin splitting.

**Note added.** After submission of this paper a preprint by Wunderlich et al. appeared reporting on an experimental observation of the spin Hall effect in $p$-doped GaAs quantum wells as studied here.

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