Disorder effects on the spin-Hall current in a diffusive Rashba two-dimensional heavy-hole system

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We investigate the spin-Hall effect in a two-dimensional heavy-hole system with Rashba spin-orbit coupling using a nonequilibrium Green’s function approach. Both the short- and long-range disorder scatterings are considered in the self-consistent Born approximation. We find that, in the case of long-range collisions, the disorder-mediated process leads to an enhancement of the spin-Hall current at high heavy-hole density, whereas for short-range scatterings it gives a vanishing contribution. This result suggests that the recently observed spin-Hall effect in experiment is a result of the sum of the intrinsic and disorder-mediated contributions. We have also calculated the temperature dependence of spin-Hall conductivity, which reveals a decrease with increasing the temperature.

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I. INTRODUCTION

Spin-Hall effect has been extensively studied in semiconductors with spin-orbit (SO) coupling due to its potential applications in the emerging field of spintronics. It refers to an appearance of the net spin current flowing perpendicular to the applied dc field. This transport phenomenon was studied by Dyakonov and Perel in 1971 and by Hirsch more recently. Therein, the authors demonstrated that the spin-dependent scattering between electrons and impurities causes the electrons with opposite spins to veer to different sides of the considered systems. Obviously, such spin-Hall effect strongly relies on the electron-disorder collision and hence, lately, has been named as extrinsic spin-Hall effect.

Recently, an impurity-free spin-Hall effect, namely intrinsic spin-Hall effect, has been proposed by Sinova et al. in two-dimensional (2D) electron systems and Murakami et al. in p-doped bulk semiconductors respectively. This spin-Hall effect is associated with the dc-field-induced transitions between the spin-orbit-coupled bands and contributes from all occupied electron states below the Fermi energy. In 2D electron semiconductors with Rashba and/or Dresselhaus spin-orbit coupling, the value of intrinsic spin-Hall conductivity has been found to be a universal value $e/8\pi$. Further, in 2D Rashba heavy-hole (HH) systems, Schliemann and Loss reported that the intrinsic spin-Hall conductivity starts out at value $9e/8\pi$ and increases with increasing the Rashba coupling.

However, the disorder can strongly affect the spin-Hall effect, especially in 2D semiconductors. There exists another collision-related spin-Hall current connecting to the electron states near the Fermi surface. It is disorder-mediated but independent of the impurity density. In diffusive Rashba 2D electron systems, this disorder-mediated spin-Hall effect leads to a complete cancellation of the total spin-Hall current for both the short- (Refs. 5, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18) and long-range disorders. The same conclusion has been obtained even in the presence of both the linear in momentum Rashba and Dresselhaus SO couplings.

Experimentally, observations of spin-Hall effect have been reported recently by Kato et al. and by Wunderlich et al. The latter work is of special interest, since there the spin-Hall effect has been found in a relatively clean 2D heavy-hole sample with Rashba spin-orbit coupling. Obviously, in such a system the observed spin-Hall effect cannot be understood as an extrinsic one. To interpret this experimental finding, it immediately arises the question whether the sum of the intrinsic and the disorder-mediated contributions to spin-Hall current also vanishes in the Rashba 2D heavy-hole semiconductors. By means of Kubo formalism, Bernevig and Zhang found that the disorder has no effect on the spin-Hall effect and the observed spin-Hall effect is a pure intrinsic one.

Based on a nonequilibrium kinetic equation approach, we demonstrate in this paper that the vanishing of the disorder effect on spin-Hall current in 2D HH systems occurs only for short-range hole-impurity scattering. When the disorder becomes long-ranged, the contribution from disorder-mediated process to the spin-Hall current can not be ignored. It has the same sign as the intrinsic one at high HH density, but opposite for low density. The comparison between theory and experiment indicates that the observed spin-Hall effect is the result of the sum of the disorder-mediated and intrinsic contributions. We also find that the spin-Hall conductivity decreases with the rise of the temperature.

The paper is organized as follows. In Sec. II the noninteracting Green’s functions in spin basis and the kinetic equations for nonequilibrium distribution functions are presented. In Sec. III we analyse the disorder effects on spin-Hall conductivity for short- and long-range hole-impurity scatterings, respectively. Finally, we conclude our results in Sec. IV.
II. FORMALISM

In bulk semiconductors like GaAs, the heavy- and light-hole (LH) bands with total angular momentum \( j = 3/2 \) are degenerate at the band edge. However, in quasi-two-dimensional semiconductors, the additional confinement along the growth direction of heterostructures yields a splitting between these bands and the degeneracy is lifted. As a result, the HH and LH subbands are separated.

We consider a two-dimensional HH system, where only the lowest heavy-hole subband is occupied. Note that this condition can be satisfied when the quasi-2D system is sufficiently narrow and the density and the temperature are not too high. In this way, the effective Hamiltonian for a single heavy-hole subjected a spin-orbit interaction due to the structural inversion asymmetry, can be written as:

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

with 2D momentum \( p \equiv (p_x \cos \phi_p, p_y \sin \phi_p) \), \( \hat{\sigma}_+ \equiv \hat{\sigma}_x \pm i \hat{\sigma}_y \), and \( p^\pm \equiv p_x \pm i p_y \). \( \hat{\sigma}_\mu \equiv (\hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z) \) are the Pauli matrices and \( m \) is the hole effective mass. Note that this Hamiltonian is obtained through the decomposition of the HH-LH coupling by third-order Löwdin perturbation theory. The parameter \( \alpha \) is proportional to the Rashba spin-orbit coupling constant, and relies on the separation between HH and LH subbands and the Luttinger parameters. We can see from Eq. (1) that the spin-orbit interaction is cubic in momentum. There exists another type of the cubic SO coupling, namely the Dresselhaus spin-orbit coupling in 2D electron systems. The spin-Hall effect for such SO interaction has already been studied in Ref. 11.

It follows from Eq. (1) that the Green’s function of non-interacting particles has the form

\[
\hat{G}_0^{\alpha,\beta}(\omega, p) = \tilde{\Pi}^{(1)} G_{01}^{\alpha,\beta}(\omega, p) + \tilde{\Pi}^{(2)} G_{02}^{\alpha,\beta}(\omega, p),
\]

with \( G_{0\mu}^{\alpha,\beta} = [\omega - \varepsilon_\mu(p)]^{-1} \) \((\mu = 1, 2)\). Here,

\[
\varepsilon_\mu(p) = \frac{p^2}{2m} + (-1)^\mu \varepsilon_{HH},
\]

\[
\tilde{\Pi}^{(\mu)} = \frac{1}{2} \left[ \delta_{\alpha\beta} + \frac{(-1)^\mu}{p} \left( p^2 \hat{\sigma}_+ \alpha_\beta - p^2 \hat{\sigma}_- \alpha_\beta \right) \right],
\]

and \( \varepsilon_{HH} \equiv \alpha p^3 \). The operator \( \hat{\Pi}^{\mu} \) represents the projection onto the states with a definite helicity.

By means of a local unitary transformation

\[
\hat{U}(p) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & i e^{3i\phi_p} \\ i e^{3i\phi_p} & 1 \end{pmatrix},
\]

the Hamiltonian \( \hat{H} \) can be diagonalized as \( \hat{H} \equiv \hat{U}^\dagger \hat{H} \hat{U} = \text{diag}(\varepsilon_1(p), \varepsilon_2(p)) \), and hence the noninteracting Green’s function also becomes diagonal \( \hat{G}_0^{r,a} \equiv \hat{U}^\dagger \hat{G}_0 \hat{U} = \text{diag}(G_{01}^{r,a}, G_{02}^{r,a}) \). This implies that the spin-orbit interaction can lead to further lifting the degeneracy of the HH band. In result, two spin-orbit-coupled bands with dispersion relations \( \varepsilon_\mu(p) \) are formed. Note that above transformation corresponds to a change of the basis of the Hilbert space from a spin to a helicity one. In the following study, the spin-Hall effect will be carried out in the helicity basis.

We assume a weak dc field \( \mathbf{E} \) applied to the 2D HH systems along the \( x \) direction. We are interested in the \( z \)-direction-polarized spin current flowing along the \( y \) direction, \( i.e. \) the spin-Hall current. It is known that the single-particle spin current operator can be defined by

\[
j_\sigma^y = \frac{3}{2e} \sum_p \hat{\rho}_{12}(p) \hat{\sigma}_\sigma^z j_y,
\]

where the factor \( \frac{3}{2e} \) reflects the angular momentum of the heavy-hole and the \( j_y \) is the electric current operator. By taking the unitary transformation, \( j_\sigma^y \) becomes non-diagonal and the net observed spin-Hall current can be expressed as

\[
J_\sigma^y = \sum_p \frac{3p_\sigma^z}{2m} \hat{\rho}_{12}(p) + \hat{\rho}_{21}(p) \cdot \mathbf{E}.
\]
with \( n_i \) being the impurity density and \( a_i (i = 1, 2, 3) \) the factors associated with the directions of the momenta, 
\[
a_1 = 1 + \cos(3\phi_p - 3\phi_k), \quad a_2 = 1 - \cos(3\phi_p - 3\phi_k), \quad a_3 = \sin(3\phi_p - 3\phi_k).
\]
The relaxation term \( \frac{\partial \rho}{\partial t} \bigg|_{\text{scatt}} \) takes a general form.  

Similar to the case of 2D electron systems, the linearized kinetic equation can be further simplified and its solution is found to comprise two terms. The first one is
\[
\rho_{12}^{(1)}(p) = \rho_{21}^{(1)}(p) = \frac{3eE \cdot \nabla_p \phi_p}{4\varepsilon_{HH}} \left\{ n_F[\varepsilon_1(p)] - n_F[\varepsilon_2(p)] \right\},
\]
and the real part of the second one takes the form
\[
\Re \rho_{12}^{(2)}(p) = \zeta(p) e \sin \phi_p \text{ with function } \zeta(p)
\]

The functions \( \Phi_\mu(E) \) connect to the diagonal distribution functions
\[
\rho_{\mu\nu}^{(2)}(p) = -\left. \frac{\partial n_F(E)}{\partial E} \right|_{E=\varepsilon_{\mu}(p)} \Phi_\mu[\varepsilon_{\mu}(p)] e E \cos \phi_p
\]
and can be given by the coupled equations,
\[
\frac{\partial \varepsilon_{\mu}(p)}{\partial p} = \frac{\Phi_\mu[\varepsilon_{\mu}(p)]}{\tau_{1\mu\mu}} + \frac{\Phi_\mu[\varepsilon_{\mu}(p)]}{\tau_{2\mu\mu}} - \frac{\Phi_\mu[\varepsilon_{\mu}(p)]}{\tau_{3\mu\mu}}, \quad (13)
\]
with \( \mu = 3 - \mu \). In these equations, \( \tau_{ij\mu} \) denote the different relaxation times
\[
\frac{1}{\tau_{ij\mu}} = 2\pi \sum_k |V(|p - k|)|^2 \Lambda_{i\mu\nu}(\phi_k - \phi_p, p, k), \quad (14)
\]
where the functions \( \Lambda_{i\mu\nu}(\phi, p, k) \) are defined as
\[
\Lambda_{1\mu\nu}(\phi, p, k) = \frac{1}{2}(1 + \cos(3\phi))(1 - \cos \phi)\delta(\varepsilon_{\mu\mu} - \varepsilon_{\nu\nu}), \quad \Lambda_{2\mu\nu}(\phi, p, k) = \frac{1}{2}(1 - \cos(3\phi))\delta(\varepsilon_{\mu\mu} - \varepsilon_{\nu\nu}), \quad \Lambda_{3\mu\nu}(\phi, p, k) = \frac{1}{2} \cos \phi (1 - \cos(3\phi))\delta(\varepsilon_{\mu\mu} - \varepsilon_{\nu\nu}) \quad \text{and} \quad \Lambda_{4\mu\nu}(\phi, p, k) = \frac{1}{2} \sin \phi \sin(3\phi)\delta(\varepsilon_{\mu\mu} - \varepsilon_{\nu\nu}).
\]

The first term in the solution of the linearized kinetic equation gives rise to an intrinsic spin-Hall conductivity \( \sigma_{HH}^{(1)} \)
\[
\sigma_{HH}^{(1)} = \frac{-9e}{16\pi m a} \int_0^\infty \frac{dp}{p^2} \left\{ n_F[\varepsilon_1(p) - \mu] - n_F[\varepsilon_2(p) - \mu] \right\}, \quad (15)
\]
in agreement with the previous study. This part of spin-Hall conductivity comes from the interband transition processes in which all holes below Fermi surface join. It is associated with the energy separation between two spin-orbit-coupled bands in helicity basis and reveals an intrinsic character: it is independent of any hole-impurity scattering. Physically, the dc field can cause an elastic transition of a hole from one band to another one when this hole gains an additional momentum from the external dc field.

The second term in the solution is associated with the transport process and only the hole states near the Fermi surface contribute. It relates to the disorder collision in a surprising way: its contribution to the spin-Hall conductivity \( \sigma_{HH}^{(2)} \) is independent of the impurity density \( n_i \) but depends on the above-defined relaxation times and hence the form of scattering matrix. We can understand the origin of the \( \sigma_{HH}^{(2)} \) as follows. When an external dc field is applied, the holes should participate in the longitudinal transport, leading to a diagonal distribution proportional to the inverse of the impurity density. At the same time, these perturbative holes also experience the impurity scattering, yielding the interband polarization. In result, the nondiagonal distribution becomes impurity-density-independent. Here the impurity plays only an intermediate role.

We should note that this disorder-mediated mechanism is physically identical with the side-jump mechanism studied recently in the investigation on spin-Hall effect. Contributions to spin-Hall conductivity from both mechanisms are independent of the impurity density but collision-related. At the same time, they all are associated with the hole (or electron) states near the Fermi surface. However, formally, these two mechanisms look different because of two different approaches. The side-jump process is carried out for a spin-orbit interaction involved in the electron-impurity scattering. It corresponds to a lateral displacement of the center of the wave-packet during the scattering and hence connects to the scattering-dependent term of the current operator. However, in our study, since the spin-orbit coupling is included in the free-hole (or free-electron) Hamiltonian, the current operator is independent of the hole-impurity collision.

The fact that the spin-Hall current consists of two parts, is similar to the well-known result of Strida as well as the recently obtained conclusion in the context of anomalous Hall effect (AHE). In the 2D electron systems magnetically or with magnetization, the off-diagonal conductivity usually comes from two terms, one of which is due to the electron states near the Fermi energy and the another one is related to the contribution of all occupied electron states below the Fermi energy.
III. RESULTS AND DISCUSSIONS

First, we consider the spin-Hall effect for the short-range disorder. In this case, the hole-impurity collision matrix has a simple momentum-independent form $V(|p - k|) \equiv u$ and the scattering is described by a single relaxation time $\tau = 1/\nu_i u^2$. It can be seen from Eq. (11) that the disorder-mediated contribution to spin-Hall current relies on function $A_{\mu \nu}$ proportional to $\sin \phi \sin(3\phi)$. When the angle integration in Eq. (7) is performed, the vanishing $s_H^{(2)}$ is obtained.

This result agrees with that of Ref. [21] in which the vanishing of disorder-related spin-Hall conductivity comes from an analogous angle-integration. However, for 2D electrons with Rashba spin-orbit coupling, the function $A_{\mu \nu}$ depends on $\sin^2 \phi$, leading to a nonzero $s_H^{(2)}$.

For long-range disorders, the additional momentum-dependence of scattering matrix produces rich novel phenomena. We have performed a numerical calculation to investigate the long-range disorder effect on the spin-Hall conductivity in a 2D GaAs/AlGaAs based heavy-hole system. Consider a Coulomb interaction between the 2D heavy-holes and the charged impurities located at a distance $s = 500 \text{Å}$ from the 2D plane: $V(p) \sim e^{-sp}I(p)$, where $I(p)$ is the form factor. In calculation, we take the effective mass $m = 0.27m_e$ (Ref. [20]) and the coupling constant $ma = 5 \text{Å}$.

In Fig. 1 the total and disorder-mediated spin-Hall conductivities are plotted as functions of heavy-hole density at zero temperature. The intrinsic spin-Hall conductivity is almost independent of HH density and has the value $9e/8\pi$, in agreement with the result in Ref. [7]. It is evident from Fig. 1 that, unlike the case of short-range disorder, here the $s_H^{(2)}$ and $s_H$ decrease with descending HH density. $s_H^{(2)}$ even becomes negative for $n_p < 2.5 \times 10^{10} \text{cm}^{-2}$ due to the sign change of the quantities $\tau_{\mu \nu}$.

For HH density of order of $10^{10} \text{cm}^{-2}$, the Fermi energy and the temperature (less than 4.2 K) become comparable. Hence, the HH spin-Hall effect should be strongly influenced by temperature. The calculation indicates that with ascending the temperature, the intrinsic spin-Hall conductivity begins with the zero-temperature value $9e/8\pi$ and descends for heavy-hole densities $n_p$ in the range $1 - 100 \times 10^{10} \text{cm}^{-2}$. However, as shown in Fig. 2(a), for the disorder-mediated spin-Hall conductivity, there exists a critical HH density $n_{pc}$ about equal to $4 \times 10^{10} \text{cm}^{-2}$. With a rise of the temperature, the $s_H^{(2)}$ increases for $n_p < n_{pc}$, while it decreases for the opposite case. However, one can see from Fig. 2(b) that the total $s_H$ always decreases with increasing temperature. This implies that the descending intrinsic spin-Hall conductivity plays a dominant role at low HH density.

Experimental study by Wunderlich et al. has been performed for heavy-hole density $n_p = 2 \times 10^{12} \text{cm}^{-2}$. At such high HH density, the value of spin-Hall conductivity remains almost unchanged for temperatures less than 4.2 K. At the same time, the disorder-mediated process
plays a positive role and its contribution to spin-Hall conductivity adds to the intrinsic one. Hence, the 2D HH systems with such a high HH density serve as good candidates for the observation of the spin-Hall effect.

To compare with the experiment, we have calculated the spin-Hall conductivity for the HH system with hole density equal to the experimental one. The Fermi energy is approximately chosen to be 17.5 meV and hence the coupling constant is \( m_\text{e} a = 2.5 \text{A} \). At \( T = 4.2 \text{K} \), we obtain the total spin-Hall conductivity \( \sigma_{sH} = 18.2 e/8\pi \). This result is independent of the impurity density, but relies on the forms of the scattering matrix. Although the spin-Hall conductivity is not a quantity directly observed in experiments, our investigation suggests that the observed spin-Hall effect may not only be a pure intrinsic one, as claimed in Ref. [21] rather comes from both the intrinsic and the disorder-mediated processes.

IV. CONCLUSION

The spin-Hall effect of a 2D heavy-hole system with Rashba spin-orbit interaction has been investigated by means of a nonequilibrium Green’s functions approach. We have studied the intrinsic and disorder-mediated contributions to spin-Hall conductivity considering both the short- and long-range hole-disorder scatterings. For short-range collisions, the disorder-mediated contribution vanishes. When impurity scattering becomes long-ranged, however, the disorder-mediated spin-Hall conductivity becomes finite and can change the sign. It is negative for low HH density and positive for high density. The temperature dependence of disorder-mediated and total spin-Hall conductivity has also been analyzed. The total spin-Hall conductivity always descends with rising temperature at different HH densities, whereas the behaviors of the disorder-mediated one versus temperature become hole-density-related. A comparison with recent experiment indicates that the observed spin-Hall effect is probably a result of the contributions from both the intrinsic and disorder-mediated processes.

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