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2010 J. Phys.: Condens. Matter 22 095803

(http://iopscience.iop.org/0953-8984/22/9/095803)

IOP PUBLISHING JOURNAL OF PHYSICS: CONDENSED MATTER

J. Phys.: Condens. Matter **22** (2010) 095803 (8pp) doi:10.1088/0953-8984/22/9/095803

Spin polarization induced by in-plane electric and magnetic fields in two-dimensional heavy-hole systems

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Received 20 September 2009, in final form 20 December 2009
Published 10 February 2010
Online at stacks.iop.org/JPhysCM/22/095803

Abstract
Using a nonequilibrium Green function approach, we systematically investigate the current induced spin polarization (CISP) in a two-dimensional heavy-hole system with cubic Rashba spin–orbit coupling, driven by in-plane electric and magnetic fields. We find that when a magnetic field is applied along the direction of electric field, the longitudinal conductivity drops monotonously with an increase of magnetic-field strength or of hole density. The spin polarization along the electric-field direction is just the Pauli paramagnetism and it quadratically increases with an increase of hole density. The nonvanishing out-of-plane component of spin polarization emerges for both short-range and long-range disorders, and it changes sign with the variation of magnetic field, especially for long-range hole-impurity scattering. In the magnetic-field dependences of this out-of-plane CISP and of the in-plane CISP perpendicular to the electric field, there are singular magnetic fields, below or above which the effects of magnetic field are completely different.

1. Introduction

Generation and control of spins in semiconductors are fundamental issues in the emerging field of spintronics [1, 2]. The conventional spin injection from ferromagnetic metal into semiconductor is not an efficient way because most of the spin polarization will be lost at the interface due to the large conductivity mismatch [3]. The discovery of current induced spin polarization (CISP) [4], which shows up as a spatially homogeneous spin polarization in two-dimensional (2D) systems due to an in-plane charge current, discloses the possibility of generation of spin polarization directly by an electric field rather than a magnetic field. It is noted that the CISP was predicted first by Dyakonov and Perel [4] in systems with spin–orbit coupling (SOC) induced by electron-impurity scattering. Recently, many novel phenomena in systems with intrinsic SOC, such as the spin Hall effect [5–8], have been observed. This stimulates a great deal of theoretical investigation on the CISP in systems with intrinsic spin–orbit interaction [9–15].

The previous theoretical research on the CISP mainly focused on the 2D electron system with $\boldsymbol{k}$-linear Rashba SOC. In this system, only the in-plane CISP component perpendicular to the electric field is nonvanishing and it is proportional to the spin–orbit splitting constant [9, 11]. Considering realistic electron–phonon and electron-impurity scattering, Wang *et al* have studied the CISP generated by the nonlinear high electric field [14]. They found that the CISP saturates at high electric field and it descends at elevated temperature. On the other hand, the previous studies on the spin Hall effect indicate that the motion of spin in systems with a SOC nonlinearly depending on $\boldsymbol{k}$ is completely different from that in linear Rashba SOC systems [15–17]. Hence, the same situation is expected for CISP. Liu *et al* investigated the CISP in the 2D hole gas with structure inversion asymmetry [15]. They found that CISP is linearly dependent on the Fermi energy for low hole density and it is suppressed or even changes its sign in the heavy doping regime. Recently, CISP for two-dimensional electron systems with a general SOC has been proposed [18]. Experimentally, the CISP was first measured by Silov *et al* in a 2D hole system [19] and later Sih *et al* observed the CISP for 2D electron gas in an AlGaAs quantum well [20].

In the last few years, many interesting phenomena about CISP have been predicted, including the resonant CISP with the application of an ac electric field [21] or a perpendicular magnetic field [22], the anisotropy of CISP with linear Rashba and Dresselhaus SOC [12], etc. It was also shown that an in-plane magnetic field can yield a nonzero out-of-plane spin polarization in a Rashba spin–orbit-coupled 2D electron gas with a nonparabolic energy band [13] or with long-range electron-impurity scattering [23]. This nonvanishing out-of-plane CISP leads to a nonvanishing spin Hall effect in the presence of an in-plane magnetic field [17, 23]. Kato *et al* experimentally observed a nonzero out-of-plane CISP with a magnetic field applied along the electric field in strained semiconductors [24]. A similar phenomenon has also been reported in n-type ZnSe at room temperature [25]. So far, theoretical investigations on out-of-plane CISP induced by an in-plane magnetic field have been carried out mainly for the linear Rashba model. Hence, a careful investigation on CISP in a 2D hole gas with an external magnetic field applied in the plane is required. It is noted that the 'spin' of a hole spinor is actually a total angular momentum and the spintronics for hole systems actually becomes the combination of spintronics and orbitronics [15, 26].

The paper is organized as follows. In section 2, the Hamiltonian and kinetic equation of a 2D heavy-hole gas with in-plane electric and magnetic fields are presented. In section 3, the CISP of a heavy-hole gas without magnetic field is derived analytically, and the conductivity and the CISP in the presence of magnetic field are evaluated numerically. Finally, a brief summary is drawn in section 4.

2. Formalism

2.1. Hamiltonian

In the absence of magnetic field, the valence band of p-doped bulk semiconductor, such as p-type GaAs, is fourfold degenerate at the Γ point and it can be described by a 4×4 Luttinger Hamiltonian $\hat{H}_{\rm L}$ [27]. When an external magnetic field is applied along the x direction, the Hamiltonian can be written as

$$\hat{H} = \hat{H}_{\rm L} + \hat{H}_{\rm Z}. \tag{1}$$

Here, $\hat{H}_{\rm Z}$ is the Zeeman energy term and it is proportional to the g-factor involving both the anisotropic and isotropic parts. However, for the typical systems considered, the anisotropic part of the g-factor is usually two orders of magnitude smaller than the isotropic part, κ, and hence the anisotropic part can be ignored [28]. Thus, $\hat{H}_{\rm Z}$ is given by

$$\hat{H}_{\rm Z} = -2\mu_{\rm B}\kappa \hat{S}_x B_x, \tag{2}$$

with $\mu_{\rm B}$ as the Bohr magneton, B_x as the strength of magnetic field, and $\hat{S}_x$ as the x-component of spin $\frac{3}{2}$ operator:

$$\hat{S}_x = \frac{1}{2}\begin{pmatrix} 0 & \sqrt{3} & 0 & 0 \\ \sqrt{3} & 0 & 2 & 0 \\ 0 & 2 & 0 & \sqrt{3} \\ 0 & 0 & \sqrt{3} & 0 \end{pmatrix}. \tag{3}$$

It is noted that, here, the concept of spin actually refers to the total angular momentum of the valence holes.

In 2D systems, the momentum k_z is quantized due to the confinement in the z direction and a gap between light- and heavy-hole bands opens at the Γ point. The gap $\Delta = 2\gamma_2\langle k_z^2\rangle/m \approx 2\gamma_2(\pi/a)^2/m$ [16, 29] (γ_2 is the Luttinger parameter and m is the mass of a free electron) depends on the confinement scale a. In a sufficiently narrow quantum well with low hole density, only the lowest subband of heavy holes is occupied at low temperature and these holes can be described by the cubic Rashba model [30, 31]. Recently, this 2D heavy-hole gas with cubic Rashba SOC has been extensively studied. In such heavy-hole systems, the spin Hall effect [29, 31–35] and spin polarization [15, 36] have been carried out theoretically, and the experimental observation of the spin Hall effect was reported [8]. Moreover, controlled spin rotation in a spin field-effect transistor setup [37] and anisotropic magnetoresistance [38] were also studied.

By means of the truncation approximation and projection perturbation method [15], the 4×4 Hamiltonian (1) reduces to a 2×2 matrix $\tilde{H}$:

$$\tilde{H} = H_{\rm R} + H_{\rm Z}, \tag{4}$$

with $H_{\rm R}$ as the cubic Rashba Hamiltonian given by

$$H_{\rm R} = \frac{k^2}{2m_{\rm h}} + {\rm i}\alpha(k_-^3\sigma_+ - k_+^3\sigma_-), \tag{5}$$

and $H_{\rm Z}$ as the Zeeman energy taking the form

$$H_{\rm Z} = -2\mu_{\rm B}\kappa \tilde{S}_x B_x. \tag{6}$$

In these equations, $m_{\rm h}$ is the effective mass of a heavy hole, α is the Rashba coefficient, $k_\pm = k_x \pm {\rm i}k_y$, $\sigma_\pm = \frac{1}{2}(\sigma_x \pm \sigma_y)$ with $\boldsymbol{k} = (k_x, k_y) = k(\cos\theta_{\boldsymbol{k}}, \sin\theta_{\boldsymbol{k}})$ as the 2D hole momentum and $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ as the Pauli matrices. The spin operators in the cubic Rashba model $\tilde{\boldsymbol{S}} = (\tilde{S}_x, \tilde{S}_y, \tilde{S}_z)$ are given by [15]

$$\tilde{S}_x = \begin{pmatrix} -S_0k_y & S_1k_-^2 \\ S_1k_+^2 & -S_0k_y \end{pmatrix}, \tag{7}$$

$$\tilde{S}_y = \begin{pmatrix} S_0k_x & -{\rm i}S_1k_-^2 \\ {\rm i}S_1k_+^2 & S_0k_x \end{pmatrix}, \tag{8}$$

$$\tilde{S}_z = \frac{3}{2}\sigma_z. \tag{9}$$

Here S_0 and S_1 are the coefficients depending on the Luttinger parameters and the material structure parameters of the heterojunction [15]. It is noted that, for narrow-gap semiconductor systems, the cubic Rashba SOC strength can be controlled by applying a gate voltage [39].

Taking the local unitary transformation

$$U_{\boldsymbol{k}} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ \mathrm{i}e^{3\mathrm{i}\chi_{\boldsymbol{k}}} & -\mathrm{i}e^{3\mathrm{i}\chi_{\boldsymbol{k}}} \end{pmatrix}, \quad (10)$$

with $\chi_{\boldsymbol{k}}$ determined by

$$\tan 3\chi_{\boldsymbol{k}} = \frac{\alpha k \sin 3\theta_{\boldsymbol{k}} - \gamma S_1 \cos 2\theta_{\boldsymbol{k}}}{\alpha k \cos 3\theta_{\boldsymbol{k}} + \gamma S_1 \sin 2\theta_{\boldsymbol{k}}}. \quad (11)$$

Hamiltonian (4) can be diagonalized and reduces to $H = \mathrm{diag}[\varepsilon_{\boldsymbol{k}1}, \varepsilon_{\boldsymbol{k}2}]$ in the helicity basis. $\varepsilon_{\boldsymbol{k}\mu}$ is the eigenenergy

$$\varepsilon_{\boldsymbol{k}\mu} = \frac{k^2}{2m_{\mathrm{h}}} + \gamma S_0 k_y + (-1)^\mu \varepsilon_M, \quad (12)$$

with $\varepsilon_M = \sqrt{\alpha^2 k^6 + \gamma^2 S_1^2 k^4 - 2\alpha\gamma S_1 k^5 \sin\theta_{\boldsymbol{k}}}$, $\mu = 1, 2$ as the helix band index, and $\gamma = 2\kappa\mu_{\mathrm{B}} B_x$. The corresponding eigenfunction is $|\boldsymbol{k}\mu\rangle = 1/\sqrt{2}[1, -\mathrm{i}(-1)^\mu e^{3\mathrm{i}\chi_{\boldsymbol{k}}}]^T$. It is noted from equation (12) that, in the presence of magnetic field, the energy spectrum of a 2D heavy-hole gas is still degenerate at the Γ point. Considering the fact that the spin operator $\tilde{S}_x$ is linearly dependent on the magnitude of the wavevector, this feature can be confirmed from the Hamiltonian (4). In contrast to this, the degeneracy at the Γ point in a 2D electron system with a $\boldsymbol{k}$-linear Rashba SOC is removed [40]. Note that the magnetic field is included in the energy spectrum $\varepsilon_{\boldsymbol{k}\mu}$ and the angle $\chi_{\boldsymbol{k}}$. The energy spectrum (12) is unstable at large wavevector due to the fact that the cubic Rashba model is valid only for small k. The lower energy branch is bounded only for

$$k \leqslant \frac{1}{6\alpha}\left[\frac{1}{m_{\mathrm{h}}} - 2\gamma S_1 + \sqrt{\left(\frac{1}{m_{\mathrm{h}}} - 2\gamma S_1\right)^2 - 12\alpha\gamma S_0}\right], \quad (13)$$

where the Zeeman energy satisfies $\gamma \leqslant \frac{1}{2S_1^2}[\frac{S_1}{m_{\mathrm{h}}} + 3\alpha S_0 - \sqrt{9\alpha^2 S_0^2 + 6\alpha\frac{S_0 S_1}{m_{\mathrm{h}}}}]$. In the absence of magnetic field, the bound condition, equation (13), reduces to the one presented in [31].

2.2. Kinetic equation

To carry out the transport quantities, such as conductivity and spin polarization, it is necessary to derive the kinetic equation for a lesser Green function. Following the procedure presented in [17] and [32], we first carry out the Dyson equations for the real-space lesser Green functions in the spin basis and then introduce the center-of-mass time, $T = (t_1 + t_2)/2$, and the relative time, $\tau = t_1 - t_2$. After that, the Fourier and the unitary transformations are performed and the equation reduces to the kinetic equation in the helicity basis. We find that, for weak in-plane dc electric field, the distribution function $\rho(\boldsymbol{k}) = -\mathrm{i}G^<(\boldsymbol{k}, T, \tau = 0)$ obeys the equation,

$$-e\boldsymbol{E}\cdot\nabla_{\boldsymbol{k}}\rho^{(0)} - \frac{3\mathrm{i}}{2}e\boldsymbol{E}\cdot\nabla_{\boldsymbol{k}}\chi_{\boldsymbol{k}}[\rho^{(0)}, \sigma_x] + \mathrm{i}\varepsilon_M[\sigma_z, \rho] = I_{\mathrm{sc}}, \quad (14)$$

with $\rho^{(0)}$ as the equilibrium distribution function,

$$\rho^{(0)} = \begin{pmatrix} n_{\mathrm{F}}(\varepsilon_{\boldsymbol{k}1}) & 0 \\ 0 & n_{\mathrm{F}}(\varepsilon_{\boldsymbol{k}2}) \end{pmatrix}. \quad (15)$$

In equation (14), $n_{\mathrm{F}}(x)$ stands for the Fermi distribution function and I_{sc} is the scattering term [41]

$$I_{\mathrm{sc}} = -\int_{-\infty}^{T} \mathrm{d}\tau' [\Sigma^> G^< + G^< \Sigma^> - \Sigma^< G^> - G^> \Sigma^<] \times (T, \tau')(\tau', T). \quad (16)$$

$G^<$ ($G^>$) and $\Sigma^<$ ($\Sigma^>$), respectively, are the lesser (greater) nonequilibrium Green functions and self-energies. In the self-consistent Born approximation, the self-energies $\Sigma^{<,>} \equiv U_{\boldsymbol{k}}^\dagger \check{\Sigma}^{<,>} U_{\boldsymbol{k}}$ ($\check{\Sigma}^{<,>}(\boldsymbol{k}, T, \tau) = \sum_{\boldsymbol{q}} |u(\boldsymbol{k}-\boldsymbol{q})|^2 \check{G}^{<,>}(\boldsymbol{q}, T, \tau)$ with $\check{G}^<$ ($\check{G}^>$) and $\check{\Sigma}^<$ ($\check{\Sigma}^>$) are, respectively, the lesser (greater) Green functions and self-energies in spin basis) are given by

$$\Sigma^{<,>}(\boldsymbol{k}, T, \tau) = \frac{1}{2}\sum_{\boldsymbol{q}} |u(\boldsymbol{k}-\boldsymbol{q})|^2 \{\Omega_{11} G^{<,>} + \Omega_{12}\sigma_x G^{<,>}\sigma_x + \mathrm{i}\bar{\Omega}_{11}[\sigma_x, G^{<,>}]\}. \quad (17)$$

Here $\Omega_{\mu\mu'} = 1 + (-1)^{\mu+\mu'}\cos(3\chi_{\boldsymbol{k}} - 3\chi_{\boldsymbol{q}})$, $\bar{\Omega}_{\mu\mu'} = (-1)^{\mu'}\sin(3\chi_{\boldsymbol{k}} - 3\chi_{\boldsymbol{q}})$, and $u(\boldsymbol{k})$ is the scattering matrix. For shortness, in the above equation the arguments $(\boldsymbol{q}, T, \tau)$ of Green functions $G^{<,>}$ are dropped.

Without loss of generality, we consider an electric field along the x direction, $\boldsymbol{E} = E_0\hat{x}$. To further simplify the scattering integral, we use the generalized Kadanoff–Baym ansatz to express the time development of a two-time Green function with its equal-time value [42] and the lowest gradient expansion is taken [43]. Finally, we find that, to the first order of electric field, the solution of equation (14) can be written as a sum of two terms, $\rho^{(1)} + \rho^{(2)}$. The first term, $\rho^{(1)}$, takes the form

$$\rho_{12}^{(1)} = \rho_{21}^{(1)} = \frac{3eE_0}{4\varepsilon_M}\frac{\partial\chi_{\boldsymbol{k}}}{\partial k_x}[n_{\mathrm{F}}(\varepsilon_{\boldsymbol{k}1}) - n_{\mathrm{F}}(\varepsilon_{\boldsymbol{k}2})]. \quad (18)$$

Ignoring the collisional broadening, the second term, $\rho^{(2)}$, is determined by equations of the form

$$-eE_0\frac{\partial n_{\mathrm{F}}(\varepsilon_{\boldsymbol{k}\mu})}{\partial k_x} = \pi\sum_{\boldsymbol{q}\mu'} |u(\boldsymbol{k}-\boldsymbol{q})|^2 \Omega_{\mu\mu'} \times [\rho_{\mu\mu}^{(2)}(\boldsymbol{k}) - \rho_{\mu'\mu'}^{(2)}(\boldsymbol{q})]\delta(\varepsilon_{\boldsymbol{k}\mu} - \varepsilon_{\boldsymbol{q}\mu'}), \quad (19)$$

$$4\varepsilon_M \mathrm{Re}\rho_{12}^{(2)}(\boldsymbol{k}) = \pi\sum_{\boldsymbol{q}\mu\mu'} |u(\boldsymbol{k}-\boldsymbol{q})|^2 \bar{\Omega}_{\mu\mu'} \times [\rho_{\mu\mu}^{(2)}(\boldsymbol{k}) - \rho_{\mu'\mu'}^{(2)}(\boldsymbol{q})]\delta(\varepsilon_{\boldsymbol{k}\mu} - \varepsilon_{\boldsymbol{q}\mu'}). \quad (20)$$

Here $\mathrm{Re}\rho_{12}^{(2)}(\boldsymbol{k})$ is the real part of the off-diagonal element of distribution function, $\rho_{12}^{(2)}(\boldsymbol{k})$. One can see that in the above kinetic equations the magnetic field is not shown explicitly. The magnetic field influences the distribution function through the energy $\varepsilon_{\boldsymbol{k}\mu}$ and the angle $\chi_{\boldsymbol{k}}$.

In the helicity basis, the spin polarization, $\boldsymbol{S} = \sum_{\boldsymbol{k}} \mathrm{Tr}[\rho(\boldsymbol{k}) U_{\boldsymbol{k}}^\dagger \tilde{\boldsymbol{S}} U_{\boldsymbol{k}}]$, can be expressed as

$$S_x = \sum_{\boldsymbol{k}\mu} [-S_0 k \sin\theta_{\boldsymbol{k}} + (-1)^\mu S_1 k^2 \sin(3\chi_{\boldsymbol{k}} - 2\theta_{\boldsymbol{k}})]\rho_{\mu\mu}(\boldsymbol{k}), \quad (21)$$

$$S_y = \sum_{\boldsymbol{k}\mu} [S_0 k \cos\theta_{\boldsymbol{k}} - (-1)^\mu S_1 k^2 \cos(3\chi_{\boldsymbol{k}} - 2\theta_{\boldsymbol{k}})]\rho_{\mu\mu}(\boldsymbol{k}), \quad (22)$$

$$S_z = 3\sum_{\boldsymbol{k}} \mathrm{Re}\rho_{12}(\boldsymbol{k}), \quad (23)$$

and the average velocity of heavy holes is given by

$$\boldsymbol{v} = \frac{1}{N}\sum_{\boldsymbol{k}\mu} \nabla_{\boldsymbol{k}}\varepsilon_{\boldsymbol{k}\mu}\rho_{\mu\mu}(\boldsymbol{k}), \tag{24}$$

with N as the hole density.

It should be noted that, in the kinetic equations presented above, the carrier-impurity scattering is taken into account in the self-consistent Born approximation and, in the impurity-density expansion of I_{sc}, only the lowest order term is considered. Hence, the derived kinetic equations are valid in the clean limit regime. Further, we assume that the electric field is weak but the magnetic field may be large.

From equation (18) we see that $\rho^{(1)}$ only contains nonvanishing off-diagonal elements. It is independent of any impurity scattering and leads to a dc-field-induced transition. The diagonal elements of $\rho^{(2)}$ are inversely proportional to impurity density, while its off-diagonal elements are independent of impurity density. Correspondingly, the x-component of CISP, S_x, can be expressed as $S_x = S_x^{(0)} + S_x^{(2)}$ with $S_x^{(0)}$ and $S_x^{(2)}$ relating to the equilibrium distribution function $\rho^{(0)}$ and impurity-related distribution function $\rho^{(2)}$, respectively. In the same manner, the y-component of CISP, S_y, can be written as $S_y = S_y^{(0)} + S_y^{(2)}$ ($S_y^{(0)}$ and $S_y^{(2)}$ rely on $\rho^{(0)}$ and $\rho^{(2)}$, respectively). However, using $\cos(3\chi_{\boldsymbol{k}} - 2\theta_{\boldsymbol{k}}) \equiv \alpha k^3\cos\theta_{\boldsymbol{k}}/\varepsilon_M$, the angle integration of wavevector $\boldsymbol{k}$ yields the vanishing of the equilibrium y-component of spin polarization, $S_y^{(0)} = 0$. Hence, the spin polarization S_y comes from a collisional process associated with the hole states near the Fermi surface. The out-of-plane z-component of CISP S_z can be expressed as $S_z = S_z^{(1)} + S_z^{(2)}$. $S_z^{(1)}$ and $S_z^{(2)}$ relate to the impurity-independent distribution function $\rho^{(1)}$ and the collision-related distribution function $\rho^{(2)}$, respectively.

From the kinetic equations (19) and (20) as well as the CISP expressions (22) and (23), it follows that the z-component of CISP, S_z, is independent of the impurity density, while the y-component of CISP, S_y, is proportional to the inverse of impurity density. Similar to the origin of disorder-mediated spin Hall conductivity [32], $S_z^{(2)}$ can be understood as the result of a disorder-mediated process.

3. Conductivity and spin polarization

3.1. Absence of magnetic field

We first examine the spin polarization of a 2D heavy-hole gas in the absence of magnetic field, considering an impurity scattering with δ-potential, $u(\boldsymbol{k}-\boldsymbol{q}) = u_0$. In this case, the quantities $\varepsilon_{\boldsymbol{k}\mu}$, ε_M, and $\chi_{\boldsymbol{k}}$ reduce to $\varepsilon^{(0)}_{\boldsymbol{k}\mu} = \frac{k^2}{2m} + \alpha k^3$, $\varepsilon_m = \alpha k^3$, and $\theta_{\boldsymbol{k}}$, respectively. From equation (19), it follows that the diagonal elements of the distribution function $\rho^{(2)}(\boldsymbol{k})$ take the form

$$\rho^{(2)}_{11}(\boldsymbol{k}) = \frac{2eE_0}{u_0^2}\frac{\Delta_1}{\frac{k_{\mathrm{f}1}}{\Delta_1}+\frac{k_{\mathrm{f}2}}{\Delta_2}}\cos\theta_{\boldsymbol{k}}\delta(\varepsilon^{(0)}_{\boldsymbol{k}1}-\varepsilon_{\mathrm{f}}), \tag{25}$$

$$\rho^{(2)}_{22}(\boldsymbol{k}) = \frac{2eE_0}{u_0^2}\frac{\Delta_2}{\frac{k_{\mathrm{f}1}}{\Delta_1}+\frac{k_{\mathrm{f}2}}{\Delta_2}}\cos\theta_{\boldsymbol{k}}\delta(\varepsilon^{(0)}_{\boldsymbol{k}2}-\varepsilon_{\mathrm{f}}), \tag{26}$$

with ε_{f} as the Fermi energy, $k_{\mathrm{f}1}$ and $k_{\mathrm{f}2}$ as the Fermi wavevectors for the 2D heavy-hole system in the absence of magnetic field, and

$$\Delta_\mu = \left|\frac{\partial\varepsilon^{(0)}_{\boldsymbol{k}\mu}}{\partial k}\right|_{k=k_{\mathrm{f}\mu}}.$$

From equation (20) we find that the off-diagonal elements of the second term of the distribution function vanish

$$\mathrm{Re}\rho^{(2)}_{12}(\boldsymbol{k}) = \mathrm{Re}\rho^{(2)}_{21}(\boldsymbol{k}) = 0. \tag{27}$$

It is noted that the vanishing of these off-diagonal elements of the distribution function leads to the spin Hall effect, which is robust against the impurity, in the cubic Rashba model [16, 32].

Substituting the obtained distribution function into equation (24), we find that the longitudinal conductivity $\sigma_{xx} = Nev_x/E_0$, takes the form

$$\sigma_{xx} = \frac{e^2}{2\pi u_0^2}\frac{k_{\mathrm{f}1}\Delta_1 + k_{\mathrm{f}2}\Delta_2}{\frac{k_{\mathrm{f}1}}{\Delta_1}+\frac{k_{\mathrm{f}2}}{\Delta_2}}. \tag{28}$$

For weak spin–orbit splitting $\alpha k^3_{\mathrm{f}1}$, $\alpha k^3_{\mathrm{f}2} \ll \varepsilon_{\mathrm{f}}$, the above longitudinal conductivity reduces to

$$\sigma_{xx} \equiv \sigma_0 = \frac{e^2\varepsilon_{\mathrm{f}}\tau}{\pi}, \tag{29}$$

with $\tau = 1/mu_0^2$ as the relaxation time. In the same manner, we can obtain the spin polarization in the absence of magnetic field:

$$S_{x0} = \sum_{\boldsymbol{k}\mu}[-S_0k + (-1)^\mu S_1k^2]\sin\theta_{\boldsymbol{k}}\rho_{\mu\mu}(\boldsymbol{k}), \tag{30}$$

$$S_{y0} = \sum_{\boldsymbol{k}\mu}[S_0k - (-1)^\mu S_1k^2]\cos\theta_{\boldsymbol{k}}\rho_{\mu\mu}(\boldsymbol{k}), \tag{31}$$

$$S_{z0} = 3\sum_{\boldsymbol{k}}\mathrm{Re}\rho_{12}(\boldsymbol{k}). \tag{32}$$

Performing the angle integral, we find that only the y-component of spin polarization is nonvanishing and it takes the form

$$S_{y0} = \frac{eE_0}{2\pi u_0^2}\frac{4\pi S_0N + S_1(k^3_{\mathrm{f}1} - k^3_{\mathrm{f}2})}{\frac{k_{\mathrm{f}1}}{\Delta_1}+\frac{k_{\mathrm{f}2}}{\Delta_2}}. \tag{33}$$

For weak spin–orbit coupling, equation (33) can be simplified as

$$S_{y0} = eE_0N\tau S_0. \tag{34}$$

It is noted that in the case of weak SOC, the expressions of conductivity and spin polarization that we obtained are in agreement with the results in the previous literature [15].

3.2. Presence of magnetic field

When an external magnetic field is applied along the x direction, the kinetic equations (19) and (20) no longer can be solved analytically. We perform a numerical calculation to study the conductivity and spin polarization in a typical 2D heterojunction with Luttinger parameters chosen from [15]. The heavy-hole density is chosen to be less than 4.0 ×

10^{10} cm^{-2}, and we set the well width $a = 8.3$ nm. The hole density is so dilute that only the lowest heavy-hole subbands are occupied. The energy gap Δ between the light-hole and the heavy-hole bands is large and hence the transitions between different hole states at low temperature can be ignored.

3.2.1. Spin orientation. In the presence of an in-plane magnetic field, the expectation value of the spin for the μth helix band, i.e. the spin orientation, reads

$$\langle \boldsymbol{k}\mu|\tilde{S}_x|\boldsymbol{k}\mu\rangle = -S_0 k \sin\theta_{\boldsymbol{k}} + (-1)^\mu S_1 k^2 \sin(3\chi_{\boldsymbol{k}} - 2\theta_{\boldsymbol{k}}), \tag{35}$$

$$\langle \boldsymbol{k}\mu|\tilde{S}_y|\boldsymbol{k}\mu\rangle = S_0 k \cos\theta_{\boldsymbol{k}} - (-1)^\mu S_1 k^2 \cos(3\chi_{\boldsymbol{k}} - 2\theta_{\boldsymbol{k}}), \tag{36}$$

$$\langle \boldsymbol{k}\mu|\tilde{S}_z|\boldsymbol{k}\mu\rangle = 0. \tag{37}$$

We see that the spin orientation is always in the x–y plane and the out-of-plane component vanishes. We define the in-plane spin orientation $\boldsymbol{\mathcal{S}}_\mu(\boldsymbol{k})$ as $\boldsymbol{\mathcal{S}}_\mu(\boldsymbol{k}) \equiv \langle \boldsymbol{k}\mu|\tilde{S}_x|\boldsymbol{k}\mu\rangle\hat{x} + \langle \boldsymbol{k}\mu|\tilde{S}_y|\boldsymbol{k}\mu\rangle\hat{y}$. From equations (35) and (36) it follows that the magnitude of in-plane spin orientation, $\mathcal{S}_\mu(\boldsymbol{k})$, is given by

$$\mathcal{S}_\mu(\boldsymbol{k}) = k\sqrt{S_0^2 + S_1^2 k^2 - 2(-1)^\mu S_0 S_1 k \cos(3\chi_{\boldsymbol{k}} - 3\theta_{\boldsymbol{k}})}. \tag{38}$$

The spin orientations for different helix bands at Fermi contours in the absence of both the electric field and scattering are plotted in figure 1. For heavy-hole systems with relatively low density and relatively small SOC, the Fermi radii of two helix bands become almost equal. In the absence of magnetic field, the spin orientations of two helix bands are perpendicular to the 2D momentum and they orient along the same direction, in agreement with the result given by Liu *et al* [15]. However, the total spin polarization vanishes. In the presence of an in-plane magnetic field applied along the x direction, spins of different helix bands orient in different directions. For the external magnetic field with magnitude $\gamma = 0.5\gamma_0$ ($\gamma_0 = \frac{\alpha k_f}{S_1}$ and it is equal to 0.195 meV for the system that we studied, $k_f = \sqrt{2\pi N}$ is the Fermi wavevector for spin degenerate systems), the magnitude of spin orientation at the Fermi contour $\mathcal{S}_1(\boldsymbol{k}_{F1})$ is greater than $\mathcal{S}_2(\boldsymbol{k}_{F2})$. The total spin polarization is along the direction of the magnetic field, indicating the Pauli paramagnetism for a 2D heavy-hole system.

Although the distinction between two Fermi contours is very small in the case that we studied, it plays a dominant role in the spin-related transport phenomena, such as the spin Hall effect [32–35] and CISP [9–15]. In the presence of both the electric field and hole-impurity scattering, the departures from equilibrium distribution for different helix bands are different, leading to nonvanishing of the y-component as well as the out-of-plane component of spin polarization.

3.2.2. Short-range scattering. We first consider the CISP and conductivity for δ-form short-range impurity scattering with relaxation time $\tau = 1$ ps. The results are shown in figures 2 and 3.

In figure 2, we plot the dependences of σ_{xx}, S_x, and S_y on the Zeeman energy γ. From figure 2(a) we see that

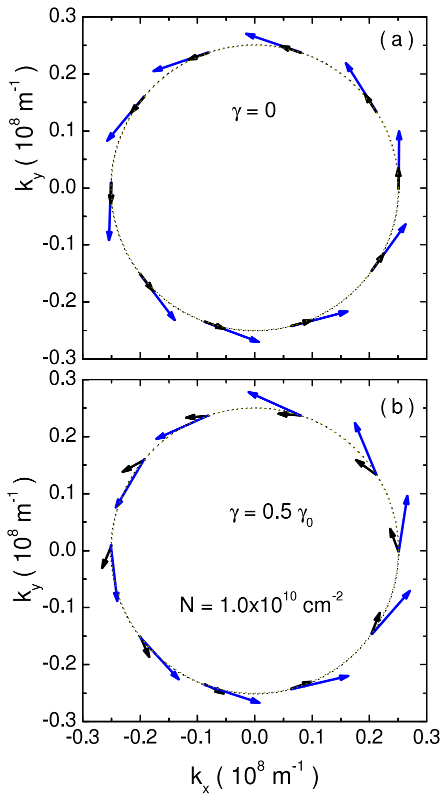

Figure 1. Spin orientations for different helix bands at Fermi contours in the absence of electric field and scattering for $\gamma = 0$ (a) and $\gamma = 0.5\gamma_0$ (b). The blue (gray) and black arrows indicate $\boldsymbol{\mathcal{S}}_1(\boldsymbol{k}_{F1})$ and $\boldsymbol{\mathcal{S}}_2(\boldsymbol{k}_{F2})$, respectively. $\boldsymbol{k}_{F1}$ and $\boldsymbol{k}_{F2}$ are two angle-dependent Fermi wavevectors in the presence of a magnetic field. The heavy-hole density $N = 1.0 \times 10^{10}$ cm^{-2}. Here $\gamma_0 = \frac{\alpha k_f}{S_1}$ and $k_f = \sqrt{2\pi N}$. For these material parameters, it is found that $\gamma_0 = 0.195$ meV.
(This figure is in colour only in the electronic version)

the longitudinal conductivity decreases monotonously with increase of the magnetic field or of the degree of doping. For S_x, numerical evaluation shows that the collision-related part $S_x^{(2)}$ vanishes and the total S_x arises from the equilibrium distribution $\rho^{(0)}$, in which all holes below the Fermi sea join. The x-component of spin polarization enhances with increase of the magnetic field or of the heavy-hole density. To lowest order of magnetic field, spin polarization S_x can be calculated analytically

$$S_x = S_x^{(0)} = \frac{\gamma}{4\pi}\left[\frac{1}{3\alpha}S_1^2(k_{f1}^3 - k_{f2}^3) + \frac{k_{f1}}{\Delta_1}(S_0 k_{f1} + S_1 k_{f1}^2)^2 + \frac{k_{f2}}{\Delta_2}(S_0 k_{f2} + S_1 k_{f2}^2)^2\right]. \tag{39}$$

For weak spin–orbit coupling, it reduces to

$$S_x = m_h N(S_0^2 + 4\pi N S_1^2)\gamma. \tag{40}$$

This S_x is the Pauli paramagnetism for the cubic Rashba model. It is noted that, in our case, the Pauli paramagnetism relies on the Luttinger parameters or on the heavy-hole spin splitting and it quadratically increases with the hole density. This is different from the Pauli paramagnetism in the $\boldsymbol{k}$-linear Rashba model

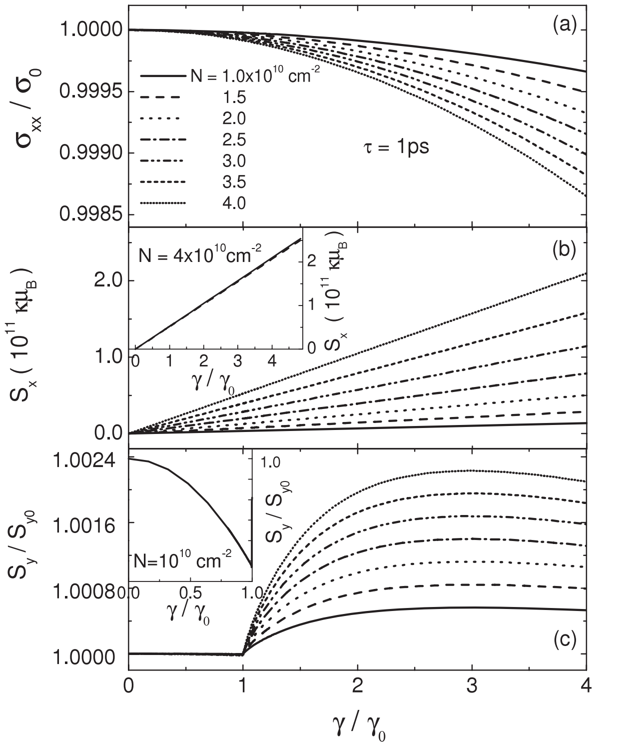

Figure 2. Magnetic-field dependences of longitudinal conductivity σ_{xx}, and the x- and y-components of spin polarization. σ_0 is the conductivity in the absence of magnetic field. S_{y0} is the y-component of spin polarization in the absence of magnetic field and it is determined by equation (34).

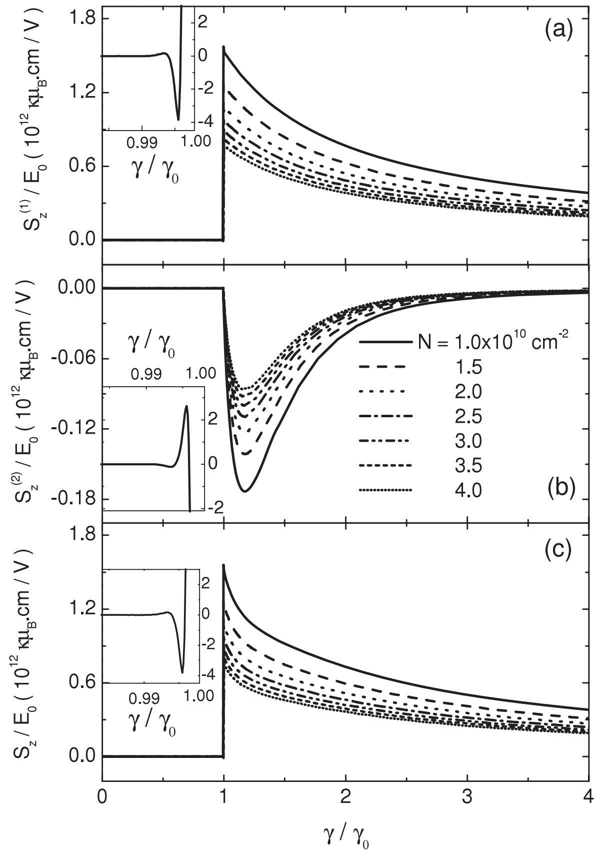

Figure 3. The impurity-independent spin polarization $S_z^{(1)}$, disorder-mediated spin polarization $S_z^{(2)}$, and the total spin polarization S_z versus magnetic field for various heavy-hole densities.

for a 2D electron system, where the Pauli paramagnetism takes the same form as that of the spin degenerate electron system and it is independent of the carrier density [13, 23]. In the inset of figure 2(b), we plot the spin polarization given by equation (40) (dash line) and the one determined by the kinetic equations (solid line). We see that for weak field, these two results coincide with each other. For large external magnetic field, a slight difference appears. The spin polarization in the x direction is just the Pauli paramagnetism, independent of the electric field. Hence, there is no CISP in this direction.

In figure 2(c), the y-component of CISP is plotted as a function of Zeeman energy. We see that this CISP component shows the magnetic-field-mediated feature, analogous to the case for the linear Rashba model [13, 23]. Obviously, there exists a singular point γ_0 for the y-component of CISP: for $\gamma < \gamma_0$, S_y is almost independent of the magnetic field, while it strongly relies on γ for $\gamma > \gamma_0$. With a rise of magnetic field from γ_0, S_y increases first and then saturates or even descends. In the inset of figure 2(c), we plot the dependence of S_y on magnetic field for $\gamma < \gamma_0$. We see that for $\gamma < \gamma_0$, S_y drops with increase of magnetic field and reaches a minimum value about $0.999\,996 S_{y0}$. The strong asymmetrical behavior of S_y below and above the singular point arises from the combined effect of an in-plane magnetic field, hole-impurity scattering and SOC, which can be understood further from figure 3.

In figure 3, the impurity-independent spin polarization $S_z^{(1)}$, disorder-mediated spin polarization $S_z^{(2)}$, and the total spin polarization S_z are plotted as functions of the magnetic field for various heavy-hole densities. We see that, for the short-range impurity scattering, all these three z-components of spin polarization do not vanish. This is different from the case in the 2D $\boldsymbol{k}$-linear Rashba model [13, 23]. In the 2D electron system with $\boldsymbol{k}$-linear Rashba SOC, the impurity-independent z-component of CISP is always zero and the disorder-mediated one exists only for long-range impurity scattering or a nonparabolic energy spectrum [13, 23]. It is noted that, in the heavy-hole systems, the disorder-unrelated out-of-plane CISP, $S_z^{(1)}$, comes from the interband transition process, which is associated with the energy separation of two helix bands and is independent of any hole-impurity scattering. All holes below the Fermi energy have probability to transit from one band to another. Hence, the nonvanishing interband polarization appears and leads to nonvanishing $S_z^{(1)}$. Therefore, $S_z^{(1)}$ possesses an intrinsic feature [44]. However, $S_z^{(2)}$ relates only to the hole states near the Fermi surface. A similar picture can be found in the studies of spin Hall effect in 2D systems with SOC [32].

From figure 3, we also see that, for external magnetic field above the singular point γ_0, $S_z^{(2)}$ is almost one order of magnitude smaller than $S_z^{(1)}$ and hence the last one plays a dominant role in the contribution to the total CISP. In the insets of figures 3(a)–(c) (where the vertical coordinate is S_z/E_0 with the units $10^{10}\kappa\mu_B$ cm V^{-1}, $10^8\kappa\mu_B$ cm V^{-1} and

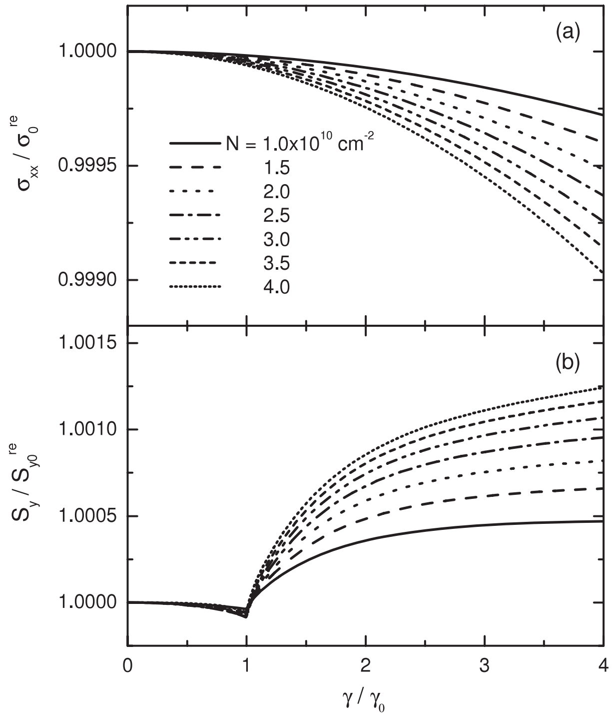

Figure 4. Longitudinal conductivity σ_{xx} and y-component of spin polarization as functions of external magnetic field for long-range impurity scattering. σ_0^{re} and S_{y0}^{re} are the conductivity and the y-component of spin polarization in the absence of magnetic field for long-range impurity scattering, respectively. $s = 100$ Å.

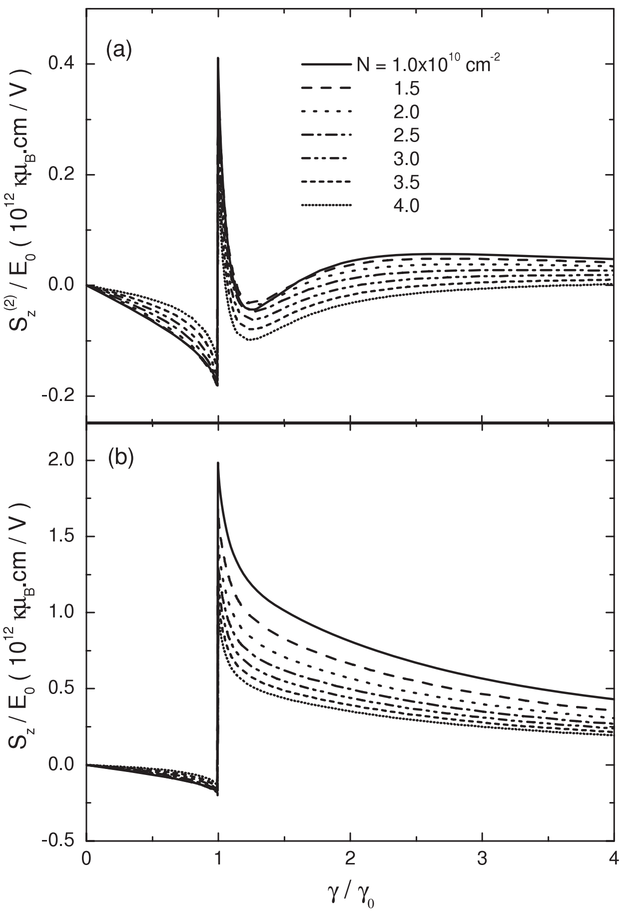

Figure 5. The disorder-mediated spin polarization $S_z^{(2)}$ and the total spin polarization S_z versus magnetic field for long-range impurity scattering.

$10^{10}\kappa\mu_{\mathrm{B}}$ cm V^{-1}, respectively), we also show the magnetic-field dependences of $S_z^{(1)}$, $S_z^{(2)}$, and S_z below the singular point for $N = 1.0 \times 10^{10}$ cm^{-2}. It is clear that the disorder-mediated CISP is two orders of magnitude less than the impurity-independent one, and the total CISP is mainly determined by the impurity-independent term when $\gamma/\gamma_0 < 1$. Near the regime of the singular point, these z-components of CISP change their signs. However, their magnitudes below γ_0 are two orders of magnitude smaller than those above the singular point. This is due to the combined effect of an in-plane magnetic field, spin–orbit splitting, and disorder on CISP. The strong distinction between the negative and positive magnitude of the CISP is in vivid contrast against the one for the 2D electron gas with linear Rashba SOC, in which S_z is an odd function with respect to the external magnetic field [13].

The existence of a singular point in the magnetic-field dependences of S_y and S_z can be understood as follows. At singular point γ_0, ε_M vanishes at the Fermi wavevector k_{f} and $\theta_{\boldsymbol{k}} = \pi/2$ for the relatively weak-SOC system. At the same time, two helix energy spectra $\varepsilon_{\boldsymbol{k}\mu}$ become degenerate and a strong interband transition process occurs. However, for the linear Rashba model, such degeneracy of energy bands does not exist for nonvanishing magnetic field [40]. Hence, in the linear Rashba model, the sudden change of the value of CISP does not occur. From equation (39), we see that S_x does not relate to the interband transition process and hence the sudden value change does not take place for S_x. For a typical heterojunction with Luttinger $\kappa = 4$ [45], the singular magnetic field is about 0.42 T, which is an ordinary magnetic field in experiment. Note that the singular point γ_0 can be used to experimentally determine the Rashba parameters: $\alpha = \gamma_0 S_1/k_{\mathrm{f}}$.

3.2.3. Long-range scattering. For long-range disorders, the additional momentum dependence of the scattering matrix may produce rich phenomena. We consider a Coulomb interaction between the 2D heavy holes and the charged impurities located at a distance s. The scattering matrix takes the form $|u(q)|^2 \simeq n_{\mathrm{i}}\mathrm{e}^{-2sq}I(q)^2$ [46], with $I(q)$ as the form factor, n_{i} as the impurity density. In calculation, s and n_{i} are chosen to be $s = 100$ Å and $n_{\mathrm{i}} = 0.15$ N, respectively.

In figure 4, the total conductivity and y-component of spin polarization are plotted as functions of magnetic field for various heavy-hole densities in the presence of long-range scattering. σ_0^{re} and S_{y0}^{re} are, respectively, the conductivity and the y-component of CISP in the absence of magnetic field for this remote hole-impurity scattering. We see that the conductivity drops with increase of the external magnetic field and of the hole density. This is similar to the case for δ-form short-range impurity scattering. For $\gamma > \gamma_0$, the dependence of spin polarization on magnetic field also has the behavior, similar to the case of short-range scattering. However, near the small regime of $\gamma \sim \gamma_0$, the spin polarization may be less than S_{y0}^{re}.

In figure 5, we plot the magnetic-field dependences of disorder-mediated spin polarization $S_z^{(2)}$ and the total spin polarization S_z in the presence of long-range impurity scattering. It is clear that the degree of asymmetry for the magnitude of the z-component of CISP below and above the singular point is suppressed. The disorder-mediated CISP below the singular point has a minus sign with the magnitude of the same order as the one above γ_0, leading to the clear negative total CISP observed in figure 5(b). It is noted that the disorder-mediated z-component of CISP, $S_z^{(2)}$, is independent of n_i.

4. Conclusions

In conclusion, the CISP for a 2D heavy-hole gas in the presence of in-plane magnetic field has been investigated. We found that the x-component of spin polarization is just the Pauli paramagnetism, independent of the external electric field, and it increases quadratically with increase of hole density. The out-of-plane spin polarization appears for both short-range and long-range disorders. It is clear that the collision-independent CISP $S_z^{(1)}$ is nonvanishing and it arises from the dc-field-induced transition between two helix bands. In the magnetic-field dependences of y- and z-components of CISP there exists a singular point, below or above which the behavior of the CISP is completely asymmetrical. However, the long-range impurity scattering can reduce the degree of this asymmetry and an evident negative z-component of CISP is obtained.

Finally, we expect that the predicted phenomena in this paper merit attempts at experimental verification by such methods as Kerr rotation [7, 24] or polarized photoluminescence technology [19].

Acknowledgments

We thank Dr H T Cui for valuable discussions. CMW and MQP gratefully acknowledge support from the National Science Foundation of China (grant No. 10947121). SYL gratefully acknowledges support from the National Science Foundation of China and from the Program for New Century Excellent Talents in University.

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