Role of relaxation in spin Hall effect

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The role of the relaxation due to the impurity scattering and/or the contacts to leads/electrodes is not taken into account23,24, or of weak disorder16,17,18,19,20,21,22, or non-equilibrium state is not taken into account23,24, or lacking a quantitative comparison with existing experiments25. Also the studies on the 4-band model which describes p-type GaAs are missing except ref.20. This is partly due to the fact that the spin relaxation is so rapid for p-holes since the SOI is much larger at the top of the valence bands compared with the bottom of the conduction bands, which has been assumed to be disadvantageous for the spin accumulation. However, the strong SOI promotes the spin current and in any case the relaxation is needed to produce the spin accumulation, which is time reversal (T)-odd, from the T-even spin current. Therefore it is a nontrivial issue which is more advantageous, p-type or n-type GaAs.

To answer all these questions, we study in this paper the Rashba and Luttinger models defined on the square lattice in terms of the Keldysh formalism applied to the finite size sample attached to the leads/electrodes26,27. These models reproduce the continuum version of each system near the Γ-point of Brillouin zone, which is most relevant for the low carrier density. The energy unit \(t\) (hopping parameter) and the length unit \(a\) (lattice constant) will be fixed later when we compare our results with experimental data. The model for the Rashba system is expressed as28

\[
H = \sum_{r,r'} c_{r\uparrow}^\dagger \tau_{rr'} c_{r'}, \quad (1)
\]

\[
t_{rr'} = \begin{cases} 
-\sqrt{1-S^2} t \mp i St_\alpha, & r = r' \pm ae_x \\
-\sqrt{1-S^2} t \pm i St_\alpha, & r = r' \pm ae_y
\end{cases} \quad (2)
\]

When the Fermi energy is near the band bottom and \(S \ll 1\), the effective mass \(m^*\) and the Rashba coupling \(\alpha\) are given by \(m^* \sim 1/(2ta^2)\) and \(\alpha \sim St_\alpha\), respectively.
The model for the Luttinger system is defined by

$$
H = \sum_{\mathbf{r}, \mathbf{r}', \mu=0}^{5} c_{\mathbf{r}\mu}^\dagger c_{\mathbf{r}'\mu} \Gamma_{\mu} \xi_{\mathbf{r}', \mu},
$$

where $\Gamma_0$ is the 4 × 4 unit matrix and other $\Gamma$-matrices are defined in ref. [5]. Assuming $p$-type GaAs thin layer, we shall take $S = 0.29, M = 2t$. This parameter set is corresponding to the typical Luttinger parameters $\gamma_1 : \gamma_2 : \gamma_3 = 6.92 : 2.1 : 2.1$ for GaAs and $(k_F a^2) = M/(2 S t) \sim 1.86$, is determined by the profile of the confined wavefunction along the z-direction [29]. In the original three-dimensional system, the kinetic terms contains $\Gamma_{1,2}$-matrices and $\Gamma_{1,2} \neq \Gamma_{1,2}$ can be approximated neglect these terms in the quasi-two-dimensional system confined in a thin layer [29]. When $t_{\gamma}' = 0$, the 4 × 4 $\Gamma$-matrix space will be decoupled to two of the 2 × 2 matrix space. However, as long as we consider the doped system, this point does not lead to any crucial difference. We shall take the units in which $\hbar = c = 1$.

For each model, we obtain the Keldysh matrix Green function by solving the integral equations numerically in the self-consistent Born approximation [28, 29]. The retarded self-energy is given by $\Sigma_{\delta \sigma}^{R}(\mathbf{r}', \delta\sigma|\delta\sigma')(\varepsilon) = \sum_{\delta\sigma'} [\Sigma_{\delta\sigma}^{R,cont}(\mathbf{r}', \delta\sigma|\delta\sigma')(\varepsilon) + \frac{\delta\sigma'}{\delta\sigma}]$, where $\Sigma_{\delta\sigma}^{R,cont}(\mathbf{r}', \delta\sigma|\delta\sigma')(\varepsilon)$ is the contact self-energy, and $\tau_{\delta\sigma}(\mathbf{r}')$ the local lifetime due to disorders. The local lifetime $\tau_{\delta\sigma}(\mathbf{r}')$ is determined self-consistently by the recursion equation, $\frac{1}{\tau_{\delta\sigma}(\mathbf{r}')}$ = $\gamma N_{\sigma}(\mathbf{r}')$, where $\gamma$ represents the strength of disorder and $N_{\sigma}(\mathbf{r}')$ is the local density of states per unit cell. The lesser Green function $G_{\delta\sigma}^{\alpha'}(\mathbf{r}', \varepsilon)$ is also determined self-consistently, by which the spatial-dependent physical quantities, i.e., the spin density/current, and charge density/current, can be calculated. We take the sample of finite size $L_x \times L_y$ with the electrodes attached at $x = \pm L_x/2$, while the open boundary condition is imposed in the $y$-direction [29]. It is noted here that the edge modes do not play crucial role in the doped case. We take the small chemical potential difference $\delta \mu / L_x = 5 \times 10^{-4} t/a$ to study the linear response regime. The chemical potential in equilibrium is taken as $\mu_0 = -3.5 t$ for the Rashba system and $\mu_0 = 0$ for the Luttinger system. Then, the Fermi energy $|\xi_F|$ measured from the band edge is $|\xi_F| \sim 0.5 t$ for the Rashba system and $|\xi_F| \sim 2t$ for the Luttinger system respectively. In both systems, the dispersion near the Fermi level is almost quadratic and isotropic. In the Luttinger system, the Fermi level is crossing only the heavy hole bands. It is noted that our models describe only the electronic states near the $\Gamma$-point in Brillouin zone but not those of whole Brillouin zone. Therefore, the above values of $|\xi_F|$ do not necessarily mean large carrier concentrations. The substantial amount of carrier concentration is determined after fixing the parameters $t$ and $a$, which will be done when we compare our results with experimental data.

![FIG. 1: Spin accumulation $\delta S_z$ and the spin current $\delta J^S_z$ in (a) and (b) the Rashba system (S=0.05) with $\gamma = 2$ (1/τ ~ 0.3t), and the Luttinger system with (c), (d) $\gamma = 1$ (1/τ ~ 0.25t) and (e), (f) $\gamma = 5$ (1/τ ~ 1.25t). The system size is $L_x \times L_y = 40a \times 40a$ for the Rashba system and $40a \times 20a$ for the Luttinger system. The chemical potential of electrons is $\mu_0 + \delta \mu/2$ at $x = L_x/2$ and $\mu_0 - \delta \mu/2$ at $x = L_x/2$. The charge current $\delta J$ (not shown) flows in the negative $x$-direction.](image_url)
the Rashba system and the spin-\(\frac{3}{2}\) matrices for the Luttinger system, and \(J_{rr'}\) is the charge current. The disorder strength is taken as \(\gamma = 2\) for the Rashba system, and \(\gamma = 1\) and 5 for the Luttinger system. Then, the inverse lifetime is \(1/\tau \sim 0.3t\) for the Rashba system, \(1/\tau \sim 0.25t\) and \(1.25t\) for the Luttinger system. Figure 2 shows (a) the spin \(z\) component \(\delta S_z\), (b) the charge current \(\delta J_x\) and (c) the divergence of the spin current \(\nabla \cdot \delta J_z\) at the \(x = 0\) cross-section, while Fig. 3 (a) the spin \(y\) component \(\delta S_y\), (b) the spin current \(\delta J_y\) and (c) the electron density \(\delta n\) at the \(y = 0\) cross-section.

As shown in Fig. 1 (a), the spin accumulation occurs all along the edges for Rashba system. This is in sharp contrast to the theoretical prediction for the Rashba system in ref. 21, where the spin current and spin accumulation is finite only near the electrodes. However since the spin current is not the conserved quantity, not all the spin current contributes to the spin accumulation. There appears sink (\(\nabla \cdot \delta J_z < 0\)), which is related to the spin torque density and the spin relaxation 30, near the negative \(y\)-edge, where the spin current is partly absorbed as shown in Fig. 2 (c). The spin accumulation comes from the remaining part of \(\nabla \cdot \delta J_z\), which is not canceled by the torque density and balancing with the spin relaxation. Therefore, the bulk SHE, the direction of the spin current and the sign of the spin accumulation are consistent.

As for the Luttinger system, the spin current is strongly enhanced near the electrodes \(x = \pm L_x/2\), but the resultant spin accumulation is rather flat along the edges \(y = \pm L_y/2\). The sign of spin accumulation pattern for \(1/\tau \lesssim t\) (\(\gamma = 1\)) is opposite to what is expected from that of spin Hall conductivity in the bulk while the direction of spin current in the bulk is consistent. This is because the spin current near the contact gives the opposite contribution in this system as shown by the profile of \(\delta J_y\) in Fig. 3 (b). When the relaxation effect is increased, the bulk property becomes dominant even in a small system and the accumulation pattern coincides with what is expected from the spin Hall conductivity. We need more rigorous argument on the definition of conserved spin current 21 in order to investigate this problem furthermore. As for the Rashba system, as seen in Fig. 3 (a), the in-plane spin accumulation \(\delta S_y\) perpendicular to the electric field is finite in the bulk as discussed in refs. 32, 33. On the other hand, there appears no in-plane spin accumulation for the Luttinger system as long as \(t_{rr'}^{L} = 0\), i.e., no hybridization between the decoupled 2 \(\times\) 2 matrix spaces in \(4 \times 4\) \(\Gamma\)-matrix space.

Next, Fig. 4 shows the inverse lifetime dependence of \(\delta S_z\). The disorder strength is taken as \(\gamma = 0.05, 0.1, 0.2, 0.5, 1, 2, 5\) and 10. Sample points are the peak values of \(|\delta S_z|\) in the region, \(|x| < 2a\) and \(|y| \sim L_y/2\). It is seen that the spin accumulation is larger for stronger SOI. This means that the magnitude of the spin current is the more important factor than the spin lifetime. Therefore, it is concluded that \(p\)-type GaAs is more advantageous than \(n\)-type to observe the spin accumulation due to the ISHE. Another observation is that the spin accumulation

![FIG. 2: Distribution of (a) \(\delta S_z\), (b) \(\delta J_x\) and (c) \(\nabla \cdot \delta J_z\) at \(x = 0\) in the Rashba and Luttinger systems. The system size is \(L_x \times L_y = 40a \times 40a\) for the Rashba system and \(20a \times 20a\) for the Luttinger system. Only the region \(y < 0\) is shown. \(\delta S_z\) and \(\nabla \cdot \delta J_z\) are the odd functions of \(y\). The disorder strength is taken as \(\gamma = 1\) (solid) and \(\gamma = 5\) (dashed) for the Luttinger system, respectively. As for the Luttinger system, \(\delta S_z\) in \(\gamma = 1\) and \(\nabla \cdot \delta J_z\) in \(\gamma = 1\) and 5 are rescaled.](image1)

![FIG. 3: Distribution of (a) \(\delta S_y\), (b) \(\delta J_y\) and (c) \(\delta n\) at \(y = 0\) in the Rashba and Luttinger systems. The system size and the disorder strengths are the same as in Fig. 2. \(\delta J_y\) of the Luttinger system is rescaled both in the cases of \(\gamma = 1\) and 5. Only the region \(x < 0\) is shown. \(\delta n\) is the odd functions of \(x\).](image2)
is rather robust against the relaxation up to $1/\tau \sim 0.1t$.

![FIG. 4: Spin accumulation as a function of the inverse lifetime. Sample points are the peak values of $|\delta S_z|$ in the region, $|x| < 2a$ and $|y| < L_y/2$. The colors are corresponding with those in Figs. 2 and 3. The sign of the accumulation pattern in the Luttinger system changes around the dashed vertical line.](image-url)

In order to compare the results with the experiment on $n$-type semiconductor, we fix $t$ and $a$ in the Rashba system as $t = 4$ meV and $a = 14$ nm. The effective mass and the carrier density is estimated as $m^* \sim 0.05m_e$ and $n_{2D} \sim 3 \times 10^{16}$ cm$^{-3}$, respectively. The Rashba spin splitting is $\Delta R \sim 5.7$S meV ($S \ll 1$). The applied electric field in our simulation is $E \sim 0.14$ mV$\mu$m$^{-1}$. In the case with $\gamma = 2$ which corresponds to $1/\tau \sim 0.3t$, the charge resistivity is $\rho_c \sim 144$ $\Omega$cm, and the spin Hall resistivity multiplied by $1/e$ is $|\rho_s| \sim 2.9 \times 10^5$, $6.4 \times 10^5$, $1.2 \times 10^4$ and $4.1 \times 10^3$ $\Omega$cm for $S = 0.01$, $0.02$, $0.05$ and $0.1$ respectively. When the results are linearly extrapolated to $E = 10$ mV$\mu$m$^{-1}$, we obtain : $|\delta J_z| \sim 70$ $\mu$A cm$^{-2}$, $|\varepsilon_0 J_z| \sim 35$, 160, 870, 2400 nA cm$^{-2}$, and $|\delta S_z| \sim 2.6$, 10, 64, 150 $\mu$A cm$^{-2}$ for $S = 0.01$, 0.02, 0.05 and 0.1, respectively. Although the Rashba coupling for $S = 0.01$ is still an order of magnitude larger than the experimental estimation of the Rashba coupling in ref. 7, $|\rho_c|$, $\delta J_z$ and $\delta S_z$ are consistently corresponding to the experimental data. However, $\rho_s$ and $\delta J_z^{2D}$ are not. This may be attributed to the spin source and sink where $\nabla \cdot \delta J_x \neq 0$. In the Luttinger system, $t$ and $a$ are fixed as $t = 10$ meV and $a = 5$ nm, which correspond to the case with $|\xi_F| \sim 20$ meV and $n_{2D} \sim 1.6 \times 10^{12}$ cm$^{-2}$. In the case with $\gamma = 1$, the charge resistivity is $\rho_c \sim 18$ $\Omega$cm. In the experiment 8, a current $I_p \sim 100$ $\mu$A is applied to the $p$-channel of $1.5$ $\mu$m width. Although we cannot exactly read the depth of the channel from the reference, it is considered to be of the order of the length unit in the model, i.e., $a = 5$ nm. In our system, this corresponds to $E_x \sim 200$ mV$\mu$m$^{-1}$. When the results are linearly extrapolated to $E_x = 200$ mV$\mu$m$^{-1}$, $|\delta S_z|/2d \sim 300$ $\mu$A cm$^{-2}$ and the spin polarization of the holes is about 2 % which is of the order of the observed circular polarization ($\sim 1$ %) of light emitted from the LED.

Finally, it is worthwhile to estimate the inverse spin Hall effect in which a gradient of external magnetic field, i.e., a spin force, induces a transverse charge current and/or electric field 51. For the linearly modulated magnetic field, $\nabla_y B_z = \text{const.}$, applied on an open system, the induced electric field is given by $|E_x| = |\sigma_{yc}^g g \mu_B \nabla_y B_z|$, where $g$ is the $g$-factor and $\sigma_{yc}^g$ is the conductivity of inverse SHE which has the relation between the spin Hall conductivity $\sigma_{yc}^S$ as $\sigma_{yc}^g = \sigma_{yc}^S / |\mu_y| \gamma$. The applied electric field is of the order of $10\mu$Vcm$^{-1}$, assuming $g \sim 2$. Although the above estimation is not large, we can enhance this inverse effect by lightly doped spin Hall insulators, i.e., materials with low carrier density and large SOI. This is because larger electric resistivity and spin Hall conductivity are advantageous for this effect.

In conclusion, we have numerically investigated the spin accumulation due to the intrinsic spin Hall effect in the Rashba and Luttinger systems by using Keldysh formalism. The distribution of the accumulated spin and the charge and spin currents are obtained, which are compared with those of the recent experiments obtaining the quantitative agreement.

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