Spatial distribution of electronic spins in a quasi-one-dimensional tight-binding model with spin-dependent hopping

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Abstract. We have theoretically studied intrinsic spin Hall effect in a quantum wire with spin-orbit interaction. Our numerical calculations show that the current-induced distribution of electronic spins has characteristic spatial dependence in a quasi-one-dimensional tight-binding model with spin-dependent hopping. The difference between the chemical potentials of electrons with up and down spins shows spatial oscillation in a direction perpendicular to the charge current and reaches the maximum around one edge and the minimum around the other edge, which suggests spin accumulation around edges of the quantum wire.

1. Introduction

In the classical Hall effect, the magnetic field induces the charge current perpendicular to the applied electric and magnetic fields. In the system of finite width, charge accumulation takes place around the edge, which produces the Hall voltage in the direction perpendicular to the current flow. We can understand what the spin Hall effect (SHE) gives rise to in a similar way. The spin-orbit interaction (SOI) in a conductor generates an effective magnetic field so that electrons with up-spin contribute to the Hall voltage as discussed above, while those with down-spin do the reverse. The induced Hall currents cancel with each other and, as a result, the Hall voltage vanishes totally. On the other hand, the counter-propagating Hall currents realize the pure spin current which is defined by the difference between them, where spin accumulation is expected around both edges. In this paper, we study the current-induced spatial distribution of electronic spins due to the SOI in a semiconductor quantum wire (QW).

The SHE can be classified into two types; one is the extrinsic SHE originating from impurity scattering which was first predicted in 1970s [1], and the other is the intrinsic SHE which originates from the electronic band structure [2, 3]. Here, we only focus on the latter and, particularly, consider the conduction band composed of a single energy band which is usually described by the Rashba model [4] within the effective-mass approximation

\[ H = \frac{p^2}{2m} + \frac{\alpha}{\hbar} (p_x \sigma_x - p_y \sigma_y), \]

where \( m \) is the effective-mass, \( p = (p_x, p_y) \) are momentum operators, \( \sigma_x, \sigma_y \) are the Pauli matrices, and \( \alpha \) denotes the coupling constant for the SOI. In the clean limit, the spin Hall conductivity was first predicted to take a universal value, \( e/8\pi \) [3]. But, soon after the prediction, it is shown to vanish regardless of the impurity scattering strength [5, 6, 7]. Here, it should be noted that it is not clear how to
define the spin current in the system with SOI where the electronic spin is not a conserved quantity and that the discussions above critically depend on the definition. Furthermore, we should pay attention to the existence of edges for finite-size systems. Actually, there are a number of reports showing non-zero values of the spin-Hall conductance, spin current flow near the edge, and spin accumulations in clean systems of various geometries [8, 9, 10].

2. Method
We consider the QW of length \( L_x \) and of width \( L_y \), and both ends are connected to electron reservoirs with chemical potentials \( \mu_L \) and \( \mu_R \), respectively, by two ideal leads which we call left and right leads in the following. To study the spatial distribution of spins, we extend Büttiker’s method [11, 12, 13] to the systems with spin-dependent voltages. In order to describe the electronic system, we use the tight-binding model with spin-dependent hopping [14]

\[
V_x C_{m-1,n} + V_x C_{m+1,n} + V_y C_{m,n-1} + V_y C_{m,n+1} = E C_{m,n},
\]

\[
V_x = (-t_0, V_{so}), V_y = (-iV_{so}, -t_0), C_{m,n} = \left( \begin{array}{c} C_{m,n}^\uparrow \\ C_{m,n}^\downarrow \end{array} \right),
\]

Here, \( t_0 \) is the hopping integral between nearest-neighbor sites, and \( V_{so} \) indicates the spin-dependent hopping, or SOI. The amplitude of the wave function at the site \((m, n)\) with spin \( \sigma \) is defined by \( C_{m,n}^\sigma \).

The dispersion relation around the bottom of the energy band in two dimension is well reproduced by the Rashba Hamiltonian \( (1) \) with the parameters, \( m = \hbar^2/(2\hbar^2) \), \( \alpha = 2V_{so}a \), and the lattice constant \( a \). In addition to the left and right leads giving the potential drop for the charge current, we attach one-dimensional (1D) ideal leads of a single conducting channel with no SOI to the sites in the QW, and prepare two reservoirs of spin-polarized electrons with the chemical potential \( \mu^\sigma \) for each site where both reservoirs are independent of each other.

Under the current flow in the \( x \)-direction from the right lead to the left one, electrons can escape to the lead attached to each site. Here, we impose the conditions that there is neither charge nor spin current through the additional lead by supplying both of spin-up and down electrons from the reservoirs. This condition is equivalent to the absence of the spin-polarized currents for both spins. What to do first is to calculate the scattering matrix (S-matrix) with respect to all the input and output channels. At zero temperature, we have only to consider the S-matrix for the Fermi energy on the assumption that the lead at site \((m, n)\)

\[
I_{mn}^\sigma = \frac{e}{h} \left\{ \sum_{\sigma'} (1 - R_{mn}^{\sigma,\sigma'}) (\mu_{mn}^\sigma - \mu_R) - \sum_{\sigma'} T_{mn,m'n'}^{\sigma,\sigma'} (\mu_{m'n'}^\sigma - \mu_R) - \sum_{\mu'} T_{mn,\text{left}}^{\sigma,\mu'} (\mu_{mn}^\uparrow - \mu_R) \right\}, \tag{4}
\]

under the unitarity of the S-matrix taken into account [16], where, \( R_{mn}^{\sigma,\sigma'} \) is the reflection coefficient in the lead at site \((m, n)\) from the input with spin \( \sigma' \) to the output with spin \( \sigma \), and \( T_{mn,m'n'}^{\sigma,\sigma'} \) represents the transmission coefficient from the input at \((m', n')\) with \( \sigma' \) to the output at \((m, n)\) with \( \sigma \). Further, \( T_{mn,\text{left}}^{\sigma,\mu'} \) denotes the transmission coefficient from the \( \mu' \)-th channel in the left lead to the lead at \((m, n)\) with spin \( \sigma \). All we have to do here is to solve the equations \( (4) \) imposing the conditions \( I_{mn}^\sigma = 0 \) for both spins at every site, which determines \( \mu_{mn}^\uparrow = \mu_R \) proportional to \( \mu_L - \mu_R \). From these spin-dependent local chemical potentials, \( \mu_{mn}^\sigma \), we define local spin polarization, or ‘local spin voltage’, as the difference \( \mu_{mn}^\uparrow - \mu_{mn}^\downarrow \) which is also proportional to the potential drop, \( \mu_L - \mu_R \).

3. Result
Density plots in Figs.1 (a) and (b) show spatial distribution of the spin voltage for the square sample with \( L_x = L_y = 100a \) and \( V_{so} = 0.1t_0 \). For both plots, the Fermi energy \( E_F = -3.54t_0 \) lies around the the
Figure 1. Two-dimensional spatial distribution of the spin voltage ($L_x = L_y = 100\alpha$, $V_{so} = 0.1 t_0$, $E_F = -3.54t_0$) for the left and right leads (a) with SOI and (b) without SOI. The cross sections at $x = 0$ for both density plots are displayed in (c).

bottom of the energy band which is well approximated by Eq.(1). The coupling constant between the 1D lead and the connected site in the QW causes incoherent scattering suppressing the phase coherence length and it is assumed to be quite weak as $10^{-3}t_0$ so as not to disturb the spin distributions.

What differs in these figures is the SOI in the left and right leads. In Fig. 1 (a), both leads generating the current flow have the same SOI as that in the QW. This means that there is no boundary at the contacts and, namely, this system is nothing but a single long QW with the SOI. So, the square region should be regarded as the part containing the sites at which the 1D lead for measuring the spin voltage is attached. Clearly, the spin distribution shows oscillations in the $y$-direction perpendicular to the current flow and the spin accumulation takes place near the edges where the direction of the spin polarization around one edge is opposite to that on the other side. Moreover, the translational symmetry appears in the $x$-direction parallel to the current flow because of the weak coupling between the QW and the lead measuring the local spin voltage.

In contrast, Fig. 1 (b) shows that oscillating behaviors also appear in the $x$-direction parallel to the current for the ideal leads with no SOI. In this case, the contacts between the QW and the ideal leads build the boundaries giving rise to the electron backward scattering, and this is why we can find the interference patterns between injected and reflected electrons. The modification of the spin distribution due to the interference might not be so small, while the spin accumulation near the edges qualitatively agrees with that in the system with no boundary as is shown by the cross sections in Fig. 1 (c).

Now, we consider the former case further to study the oscillations in the direction perpendicular to the current for the system of larger width. Considering the translational symmetry, we can minimize $L_x$, which makes it possible to investigate the system of larger $L_y$. Figures 2 (a) and (b) show the spatial distribution of spin voltages in the $y$-direction for (a) $E_F = -3.539t_0$ and (b) $E_F = -1.991t_0$ in the system with $L_y = 512\alpha$. Basically, the spatial variation is characterized by the Fermi wavelength, and the rapid oscillation appearing in the case (b) reflects the shorter wavelength than that in the case (a). It is clear that the spin voltage reaches its maximum near the edge, and we can expect that the spin accumulation survives even after taking its spatial average for the Fermi energy around the band bottom. On the other hand, it seems hardly possible to observe any spin voltages for the system with larger Fermi energy because its smaller intensity would be reduced further by the averaging the rapid oscillations.

Finally, we discuss the Fermi energy dependence of the spin accumulation in detail. To decrease the Fermi energy tends to enhance the spin accumulation around the edges and this is the case with the previous examples (a) $E_F = -3.539t_0$ and (b) $E_F = -1.991t_0$. But, the dependence is not monotonous reflecting the quasi-one dimensionality of the QW. Figures 2 (c) and (d) show the spin distributions
around the edge for the systems with the Fermi energy which is slightly smaller than that for (a) and (b) where the number of channels in the QW remains fixed. It is obvious that similar spatial variation appears in the positive voltage side, while there is no region showing negative spin voltage. This interesting behavior showing positive-definite spin voltage around the edge can be confirmed for the Fermi energy lying above the bottom of each conduction subband.

4. Summary
We theoretically studied the current-induced spatial distribution of the spin voltage in a clean QW with SOI by solving the quantum scattering problem based on a tight-binding model. For smaller Fermi energy, or lower carrier density, the spin voltage reaches its maximum around the edges and, in particular, the spin accumulation can clearly be expected for the Fermi energy lying above the bottom of a subband.

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