Numerical study on spin Hall effect for the Rashba model in a dirty limit

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Abstract. We study the impurity scattering in the spin Hall effect. The spin Hall conductance is numerically calculated by the tight-binding model with the Rashba spin-orbit coupling. In a dirty limit, the spin Hall conductance is proportional to the square of the elastic scattering time as long as the diffusive conduction is realized.

1. Introduction
A large number of studies have been done on the intrinsic spin Hall effect since the publications of two papers: One is for p-type semiconductors[1] and the other for n-type ones in two-dimensional heterostructures[2]. Experimental confirmations of the spin Hall effect were reported soon after the theoretical predictions[3, 4], while it is pointed out that the spin Hall conductance (SHC) defined by the Kubo formula vanishes in the Rashba model with δ-function-type impurities for n-type semiconductors after the vertex corrections are taken into consideration[5, 6]. However, this does not mean that SHC should vanish in any electronic systems with spin-orbit interaction. Rather, the cancellation by the vertex corrections is due to the existence of a special symmetry in the Rashba model and, actually, a nonzero value of the SHC remains unchanged in the p-type semiconductors after the vertex corrections are explicitly taken into account[7]. Disputes have not been settled even for the Rashba model, for the random potential with nonzero interaction range and the finite momentum lifetime τ might change the situation[8].

In this paper, we study effects of the impurity scattering for the SHC in a two-dimensional n-type system with a simple tight-binding model with the Rashba spin-orbit coupling. This paper is organized as follows. In Sec. 2, we give a brief introduction of the tight-binding model and the calculation method of the SHC, and numerical results are shown in Sec. 3. Concluding remarks are given in Sec. 4.

2. Model
Recent numerical studies have revealed that the tight-binding model with the Rashba spin-orbit coupling gives a nonzero SHC in the junction with four ideal leads attached. Contrary to the predictions for the intrinsic spin Hall effect, the value of the SHC is not universal, or rather dependent on the Fermi energy and the disorder due to the impurity scattering[9, 10]. In this study, we use the same model as that in the Ref. [10]. A two-dimensional square lattice of $N \times N$ sites is prepared and we call it a scattering area. A four-terminal junction is constructed by...
attaching four ideal leads with $N$ sites in width to each side of the finite-size square scattering area. The Schrödinger equation for an electron with the energy $E$ is given by

$$EC_{m,n} = \varepsilon_{m,n}C_{m,n} + V_x C_{m+1,n} + V_y C_{m-1,n} + V_g C_{m,n+1} + V_g C_{m,n-1}$$

$$C_{m,n} = \left( \begin{array}{c} C_{m,n}^1 \\ C_{m,n}^2 \end{array} \right), \quad V_x = \left( \begin{array}{cc} -t_1 & V_{so} \\ V_{so} & -t_1 \end{array} \right), \quad V_y = \left( \begin{array}{cc} -t_1 & -iV_{so} \\ -iV_{so} & -t_1 \end{array} \right),$$

where $C_{m,n}^{1(2)}$ is the amplitude of an electron with up (down) spin at the site of $(m, n)$, $t_1$ gives the hopping energy between nearest-neighbor sites, and $V_{so}$ shows the spin-orbit interaction. This model is nothing but what we called the Ando model that is widely used in the localization problem related to the symplectic symmetry\[11\] and corresponds to the Rashba Hamiltonian for the two-dimensional n-type semiconductors within the effective-mass approximation around the crossing point of two-bands with spin up and down.

Further, it is the spin-independent hopping $t_2$ between next-nearest-neighbor sites that we add to the Hamiltonian in order to remove the accidental symmetry causing the cancellation of SHC by the vertex corrections as mentioned before, while this model might be a toy model as no spin-orbit coupling is given in the additional term.

What is annoying us in the calculation of SHC by the Kubo formula is that the spin-current operator cannot be uniquely determined since the spin-orbit interaction breaks the conservation of the spin. On the other hand, we can divide the charge current into the spin-polarized components outside the scattering area by adding the two ideal leads without spin-orbit coupling perpendicular to the static charge current, and this is why such a problem with respect to the definition of the spin current is absent in this study. We solve the Schrödinger equation (1) and calculate the S-matrix so as to obtain the SHC, $G_{sH}$, by the Landauer-Büttiker formula.

### 3. Results

To study the impurity scattering, we introduce the random on-site potential $\varepsilon_{m,n}$ uniformly distributed between $[-W, W]$ in the scattering area, while $\varepsilon_{m,n} = 0$ in each lead. The scattering probability is proportional to $W^2$ and the momentum lifetime $\tau$ due to the impurity scattering is proportional to $W^{-2}$. In the following results, the configuration average is taken over about 1000 samples to obtain the transport coefficients, and the spin-orbit coupling is fixed as $V_{so} = 0.5t_1$.

Figure 1 shows the Fermi energy $E$ dependence of the SHC $G_{sH}$ for various scattering amplitudes $W$ in the absence of $t_2$, and these results are in good agreement with those in Ref. [10]. Figure 2 shows the same dependence of the SHC in the presence of $t_2 = 0.4t_1$. It is the additional hopping $t_2$ that breaks the particle-hole symmetry. On the whole, we do not find any notable universal behavior, and it is noticeable that even the sign change can take place in a strong-scattering regime, especially for the latter model. Furthermore, we faced another puzzling phenomenon. The diagonal conductance $G_{xx}$ turned out to be proportional to $W^{-2}$ even in a strong scattering limit. As is discussed in the Ref. [10], all the electronic states are localized in the thermodynamic limit $N \to \infty$ when $W$ is larger than the critical value, $W_c \approx 6.3t_1$, and the diagonal conductance shows exponential decay reflecting the Anderson localization when the system size becomes larger than the localization length. In contrast, the conductance we obtained here shows that the diffusive regime, where $G_{xx} \propto \tau$, survives for $W > W_c$.

We suppose that these intriguing phenomena originate from the conjecture that an electron can realize a diffusive conduction through the corner part of the scattering area from one lead to another lead in the perpendicular direction no matter how strong the scattering intensity is. So, in order to remove the possibility of such electron escape from strong impurity scattering peculiar to this four-terminal configuration, we also distribute the random impurity potentials in the leads, particularly, in its narrow edge region of $N \times N_e$ sites connected to the scattering area.
Figures 1 and 2 renew the results of Figs. 1 and 2 by introducing the random impurities in the connected region of each lead. Clearly, the disorder in the contact regions generates contact resistance so that the SHC is reduced. Moreover, we can see that the contact resistance eliminates the sign change of the SHC in almost all the parameter regions within the accuracy of numerical calculations.

Figure 3 shows the $W$ dependence of $G_{sH}$ at the fixed Fermi energy $E = -2t_1$ for the model with random impurities added to the connected regions. The SHC is proportional to $W^{-4}$ for $2t_1 \lesssim W \lesssim W_c$. In other words, the SHC scales as the square of the momentum lifetime $\tau$, or, $G_{sH} \propto \tau^2$ in a dirty limit as long as the system stays in the diffusive regime. This behavior shows little dependence on the value of $t_2$. In addition, our numerical results show that the SHC scales as $\Delta^2$ so. As a consequence, we can define a dimensionless parameter $\xi = \Delta \tau^2 / h$ and expect that the SHC in a dirty limit is proportional to the square of it, namely, $G_{sH} \propto \xi^2$. This
4. Concluding remarks

We have calculated the SHC of a finite-size two-dimensional square lattice with Rashba spin-orbit coupling in a four-terminal configuration by a tight-binding Hamiltonian containing random on-site potentials. To simply connect ideal leads to the square lattice might give rise to some artifact due to the possibility that electrons can escape from an ideal lead to another one passing through the corner part of the scattering area. Therefore, so much care about the contact to the ideal lead should be taken when we calculate the transport coefficients in the four-terminal configuration by using a lattice system of small size. We introduce random potentials around the connecting regions of the leads to avoid such an artifact.

Consequently, the SHC is proportional to the square of the product of the momentum lifetime and the spin-orbit coupling in a dirty limit as long as the diffusive conduction is realized. This relation remains qualitatively unchanged for the model to which the hopping term is added between next-nearest neighbor sites. The SHC of the Rashba model in the four-terminal configuration can generate a nonzero spin current in the direction perpendicular to the voltage drop, while the value of the SHC is neither so large nor universal.

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