Numerical Study of the Spin-Hall Conductance in the Luttinger Model

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We present the first numerical studies of the disorder effect on the recently proposed intrinsic spin-Hall conductance in a three dimensional lattice Luttinger model. The results show that the spin-Hall conductance remains finite in a wide range of disorder strength, with large fluctuations. The disorder-configuration-averaged spin-Hall conductance monotonically decreases with the increase of disorder strength and vanishes before the Anderson localization takes place. The finite-size effect is also discussed.

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A primary goal of spintronics is to make use of spin degrees of freedom of electrons in future “electronic” devices [1,2]. The spin-Hall effect (SHE) may be one of the potentially effective ways to manipulate the spin transport. An extrinsic SHE generated by impurities with spin-orbit (SO) coupling has been previously proposed [3]. By scattering electrons of different spins into different directions, a net spin current can be established in the transverse direction, accompanying the charge current induced by an applied electric field. But usually the resulting spin accumulation is very weak as it crucially depends on the impurity concentration. Recently, a much stronger SHE due to the intrinsic SO coupling in clean materials has been proposed for both the 3D p-doped semiconductors described by the Luttinger model [4], and the two-dimensional (2D) electron gas described by the Rashba model [5]. Here it has been argued that the “dissipationless” spin currents can be of several orders of magnitude larger than in the case of the extrinsic SHE. A signature of spin polarization observed recently in the 2D hole gas (2DHG) [6] and 3D n-doped semiconductors [7] might originate from the intrinsic SHE [8,9].

However, the effect of disorder on the intrinsic SHE remains a highly controversial issue. It has been argued [10,11] that the spin current in the 2D Rashba model should vanish, even in the weak disorder limit, after considering the vertex corrections. On the other hand, it is shown that the vertex correction vanishes for the Luttinger [12] and 2DHG [8] models such that the SHE is robust in the latter models at least when disorders are weak. Clearly,

\[
H = -\sum_{\langle ij \rangle} (c_i^\dagger c_j^\ddagger + \text{H.c.}) + V_L \sum_{\nu} (c_i^\dagger S^\nu c_{i+\nu} + \text{H.c.}) + \frac{V_L}{8} \sum_{\nu, \mu} c_i^\dagger \{S_\mu, S_\nu\} (c_{i+\mu+\nu} + c_{i-\mu-\nu} - c_{i+\mu-\nu} - c_{i-\mu+\nu}) + \sum_i \epsilon_i c_i^\dagger c_i,
\]

where the electron annihilation operator \(c_i\) has four components characterized by the “spin” index \(S = \frac{1}{2}, \frac{1}{2}, -\frac{1}{2}, -\frac{3}{2}\) respectively, and \(i + \nu (\nu = x, y, z)\) denote the nearest neighbors of site \(i\), and \(i + \nu + \mu, \text{etc.},\) for the next nearest-neighbor sites. Here \(V_L = \frac{2y_z}{\gamma_{1/2}}\) represents the strength of the Luttinger spin-orbital coupling. We choose \(V_L = 0.364\) as the ratio \(\gamma_1/\gamma_2\) is around 3 in typical semiconductors [17]. The last term accounts for on-site nonmagnetic disorder with \(\epsilon_i\) randomly distributed within \([-W/2, W/2]\). Note that the Luttinger model is only a valid description of real semiconductors around the \(\Gamma\) points at \(k_x \rightarrow 0\), which corresponds to choosing the band edge in the present tight-binding version.

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The SHC for each disorder configuration can be calculated by the Kubo formula [18]

$$\sigma_{SH}^1 = -\frac{2}{N_L} \text{Im} \sum_{E_n < E_f < E_m} \frac{\langle n | j^{\text{spin}} | m \rangle \langle m | j^{\text{spin}} | n \rangle}{(E_m - E_n)^2},$$

(2)
in which $N_L$ is the number of lattice sites, $E_f$ denotes the Fermi energy, $E_{m,n}$ is the eigenenergy, the charge current operator $j = e \mathbf{v}$, and the spin current $j^{\text{spin}}_{\mu} = \frac{1}{2} \langle \sigma_{\mu} \mathbf{S} \rangle$. Here the velocity operator $\mathbf{v}$ as the conjugate operator of the position operator $\mathbf{R} = \sum_{i \sigma} r_{i \sigma}$, $(n_{i \sigma})$ is the number operator at site $i$ with spin index $\sigma$, is defined by the standard relation $\mathbf{v} = \frac{i}{\hbar} [\mathbf{H}, \mathbf{R}]$. In the presence of random disorder $W \neq 0$, the SHC is obtained by averaging $\sigma_{SH}^1$ over all disorder configurations, i.e.,

$$\sigma_{SH} = \langle \sigma_{SH}^1 \rangle.$$

(3)

In a finite-size calculation, a proper boundary condition (BC) is necessary for diagonalizing the Hamiltonian. A general (twisted) BC, e.g., $\psi(x + L_x, y, z) = e^{2\pi i x / L_x} \psi(x, y, z)$, etc., where $L_x$ is the sample size along the $x$ direction, and $\phi_x$ is defined within $[0, 1]$ with $\phi_x = 0$ corresponding to the periodic BC (PBC) along this direction. In the thermodynamic limit, a physical quantity should not depend on BCs. In a finite-size calculation, the BC averaging can be very effective in smoothing out finite-size fluctuations in $\sigma_{SH}$ in a spin-orbit coupling system [16]. In principle, this procedure is not necessarily the unique one for a finite system (as one can also use the fixed BCs in the calculation), but smoother data obtained this way can allow one to make a finite-size scaling analysis and to meaningfully extrapolate the results in the thermodynamic limit. For example, let us first consider the PBC in the pure system with $\epsilon_j = 0$. The calculated $\sigma_{SH}$ for an $8 \times 8 \times 8$ lattice is shown in Fig. 1 by the dashed curve, which quickly fluctuates, as a function of $E_f$, with finite steps due to the finite-size effect. Such a finite-size effect disappears when the sample size is increased to $50 \times 50 \times 50$ (this size can only be reached for the pure system, where the momentum is a good quantum number, in our calculation) with the same PBC, as indicated by the smooth solid curve in Fig. 1. On the other hand, if one averages over different BCs (over 200 configurations) in Eq. (3) for the $8 \times 8 \times 8$ lattice, the steps in the dashed curve can also become smoothed out as represented by the open circles which coincide very well with the solid curve obtained for the bigger lattice of $50 \times 50 \times 50$ in Fig. 1.

The fluctuations in $\sigma_{SH}^1$ become very large in the presence of disorders, typically in a range of 5–10 times larger than the averaged value. To quantitatively describe such fluctuations, we shall introduce the so-called distribution of the SHC (DSHC), $P(\sigma_{SH}^1)$, which determines the averaged SHC, $\sigma_{SH}$, by

$$\sigma_{SH} = \int d\sigma_{SH} P(\sigma_{SH}^1) \sigma_{SH}^1.$$

(4)

First, for a given $E_f$, we can calculate $\sigma_{SH}^1$ at different disorder and BC configurations within a small Fermi energy interval, say, $[-2.27, -2.07]$ around $E_f = -2.17$ as illustrated in Fig. 1 by the arrow [here the change in $\sigma_{SH}(E_f)$ is presumably weak as a function of $E_f$]. Suppose that the total number of computed $\sigma_{SH}^1$’s is $N$ in this range, and the number of $\sigma_{SH}^1$’s at $\sigma_{SH} = \sigma \pm \Delta \sigma$ [$\Delta \sigma = \pm 0.01(e/8\pi)$], is denoted by $\Delta N(\sigma)$. Then the DSHC is defined as the statistic distribution of $\sigma_{SH}^1$

$$P(\sigma) = \frac{\Delta N(\sigma)}{N \Delta \sigma}.$$

(5)

The DSHC for the pure system of an $8 \times 8 \times 8$ lattice for 200 different BCs is shown in the inset of Fig. 1, in which $P(\sigma)$ is a very symmetric peak such that one may simply use the peak position, $\frac{1}{2} \sigma_{\text{av}}$, to determine the averaged $\sigma_{SH}$ instead of directly evaluating the average in Eq. (4). A similar technique has been used in the quantum Hall effect system [19].

Figure 2(a) shows the DSHC at $W = 3$ for a $6 \times 6 \times 6$ lattice, with the Fermi energy $E_f$ fixed as the same value as in Fig. 1. Here the open squares correspond to the result obtained over $N = 1000$ configurations of random disorder and BCs, while the closed squares are for the $N = 5000$ configurations. Clearly, the DSHC becomes smoother with the increase of $N$, whose symmetric peak position remains unchanged with essentially the same envelope. The solid curve in Fig. 2(a) is obtained by averaging the DSHC at $N = 1000$ over a small range of $\sigma$: $[\sigma - \delta, \sigma + \delta]$ with $\delta = 0.2 (e/8\pi)$, defined by $P_d(\sigma) = \frac{1}{2\delta} \int_{\sigma-\delta}^{\sigma+\delta} d\sigma' P(\sigma')$, which coincides with the data at $N = 5000$ very well and is plotted in a wider range of $\sigma$ in the inset. The calculated $P_d$ at $W = 0.0, 0.4, 3.0$, and 10, respectively, for an $8 \times 8 \times 8$ lattice averaged over 200 configurations is presented in Fig. 2(b). The main panel focuses on the neighborhood
FIG. 2. (a) The DSHC at \( W = 3 \) on a \( 6 \times 6 \times 6 \) lattice. Open squares denote 1000 random disorder and BC configurations, and closed squares are for 5000 configurations. The solid curve is the averaged DSHC, \( P_a \) (defined in the text), at 1000 configurations. The inset shows \( P_a \) in a larger scale. (b) \( P_a \) at different disorder strengths. The dotted curve is for \( W = 0 \); the solid curve \( W = 0.4 \); the dashed curve \( W = 3 \); the dash-dotted curve \( W = 10 \). Inset: the same curves in a larger scale.

around the peaks of \( P_a(\sigma) \) and the inset illustrates the peaks in a larger scale, whose line shapes are generally symmetric such that one may read off the value of \( \sigma_{SH} \) directly from the peak position as discussed above.

Now we study the sample-size dependence of the SHC with the focus on three disorder strengths: \( W = 0.4 \) for the weak disorder regime, \( W = 3 \) for the intermediate regime, and \( W = 10 \) for the strong disorder regime. The results for \( W = 0.4 \) are plotted in Fig. 3(a) for three different sizes of the lattice: \( 6 \times 6 \times 6 \) with \( N = 500 \) (solid curve), \( 8 \times 8 \times 8 \) with \( N = 200 \) (dashed curve), and \( 10 \times 10 \times 10 \) with \( N = 200 \) (dotted curve). In Fig. 3(b) the difference between the \( 6 \times 6 \times 6 \) and \( 10 \times 10 \times 10 \) lattices is also presented. As the integrated \( P_a \) is normalized to unit for all sizes, the \( P_a \) at \( 10 \times 10 \times 10 \) has a relatively much longer tail such that \( \Delta P_a \) in Fig. 3(b) remains negative over a wide range of \( \sigma_{SH} \) that is not easily seen by the naked eye. These results show that the peak of \( P_a(\sigma_{SH}) \) is significantly broadened and reduced with the increase of the sample size, thus the fluctuations may survive in the large system size limit, like near the critical point of a quantum Hall system [19]. Such large fluctuations of the SHC may be attributed to the nonconserved spins under the random scattering of disorder. However, the peak position remains essentially unchanged, which still well decides the averaged \( \sigma_{SH} \). On the other hand, much less sample-size dependence is found for \( W = 3 \) and \( W = 10 \), corresponding to two peaks in Fig. 3(c), respectively, where the data for different sample sizes all coincide with each other. The differences of the DSHCs between the \( 6 \times 6 \times 6 \) and \( 10 \times 10 \times 10 \) lattices are shown in Fig. 3(d), which are indeed much reduced as compared the weak disorder case in (b).

To further characterize the size dependence of \( P_a \) and \( \sigma_{SH} \), we use a function \( \frac{1}{|\sigma_{SH}-\sigma_{SH}|^{1+c}} \) to fit \( P_a \), in which the typical width of the DSHC, \( \Delta \sigma_{SH} \), defined as the half width half maximum (HWHM), is given by \( c_{1/b} \), and two examples of the good fitting are shown in the insets of Figs. 3(a) and 3(c) for a \( 10 \times 10 \times 10 \) lattice. In this way we can systematically determine both \( \sigma_{SH} \) and the corresponding \( \Delta \sigma_{SH} \) at different sample sizes and disorder strengths. The results are depicted in Figs. 4(a) and 4(b) as functions of the disorder strength \( W \). In the weak disorder regime, we see that \( \sigma_{SH} \) remains almost the same as the pure system. With the increase of \( W \), \( \sigma_{SH} \) decreases monotonically and is reduced to 5% of the disorder-free value at \( W \sim 10 \). It becomes indistinguishable from zero.
around $W \sim 14$, which is quite close to the typical critical disorder strength, $W_c \sim 16$ [20], of the Anderson localization in 3D systems as marked in the inset of Fig. 4(a). So the results suggest that the SHE always occurs in the delocalized regime below $W_c$. Furthermore, the finite-size effect is very weak at $W \geq 2$, from $6 \times 6 \times 6$ to $10 \times 10 \times 10$, with the continuous reduction of $\Delta \sigma_{\text{SH}}$ [Fig. 4(b)].

The overall fluctuations of the SHC and the sample-size dependence are the strongest in the intermediate regime of $0.5 < W < 2$. Both effects are then monotonically reduced at $W \geq 2$, where $\sigma_{\text{SH}}$ becomes weakly dependent on the sample size and the relatively small $\Delta \sigma_{\text{SH}}$ also indicates the reduction of intrinsic fluctuations at larger $W$. These results suggest that there may exist a characteristic length scale in the spin transport which decreases with the increase of $W$. If this is true, then the extrapolation to the thermodynamic limit should be at least reliable in the strong disorder regime for the present finite-size calculation. By a simple interpolation between the pure case and the strong disorder case, then the SHC is expected to be robust over a wide range of disorder strength.

In conclusion, we numerically studied the distribution of the spin-Hall conductance and determined the SHC. The main result shown in Fig. 4 indicates that in the weak disorder regime $\sigma_{\text{SH}}$ remains almost the same as the value for the pure system. With the increase of the disorder strength, $\sigma_{\text{SH}}$ is reduced and terminates before the 3D Anderson localization takes place. Although the calculation has been performed on finite lattice sizes, through the finite-size analysis of the distribution function of the SHC, we found that the results are quite size independent, suggesting that the SHC in the 3D Luttinger model be robust. This is in contrast to the vanishing behavior found in the 2D electron Rashba model, in agreement with analytical results considering vertex corrections [11,12].

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