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Numerical simulation of diffusive conductivity in Rashba split two-dimensional gas

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Abstract

We numerically model the conductivity of a two-dimensional electron gas (2DEG) in the presence of the Rashba spin–orbit (SO) interaction in the diffusive transport regime. We performed simulation using samples which width W and length L are up to 200 and 30 000, respectively, on a tight-binding square lattice. When the system is in the diffusive regime, the quadratic increase of the conductivity with SO interaction strength λ_{SO} derived previously by Born approximation is reproduced except for very weak SO interaction. In order to obtain satisfactory agreement between numerical and analytical results, the sample width and length should be much larger than the mean free path ℓ but the length should be shorter than the localization length ξ, e.g. $4\ell \lesssim W$ and $10\ell \lesssim L \ll \xi$. The anomaly at weak SO interaction is also observed in the conductance fluctuation and the localization length, and is attributed to the finite size crossover from symplectic to orthogonal class with decreasing SO interaction. The typical values of the SO interaction characterizing the crossover obtained for $\ell \sim 48$ are $\lambda_{SO} \sim 1.0/W$ and $0.2/W$ when we impose open and periodic boundary conditions, respectively.

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Keywords: Rashba spin–orbit interaction; Diffusive conductivity; Numerical simulation; Universality class

1. Introduction

Spintronics is the rapidly developing field of research aiming to use not only the charge but also the spin degree of freedom of electrons in electronic circuits and devices [1]. As compared with several methods to utilize the spin degree of freedom such as ferromagnetic semiconductors and semiconductor/ferromagnet junctions, use of an intrinsic magnetism in semiconductors by way of the spin–orbit (SO) interaction appears very attractive. In non-magnetic conductors with sufficiently strong SO interaction, a spin polarization can be created simply by applying a source-drain bias [2–7]. The two-dimensional electron gas (2DEG) is an ideal model system to investigate the physics of these effects. In sufficiently asymmetric confinement potentials, the so-called Rashba term dominates the SO interaction [8]. Datta's spin transistor concept [9] is based on the tunability of the Rashba interaction by an external gate potential [10].

Recently, the longitudinal conductivity, spin accumulation and spin Hall conductivity have been derived for the Rashba 2DEG in the diffusive regime [5,11]. The longitudinal conductivity σ has been found to increase quadratically with increasing SO interaction strengths λ

$$\sigma = \sigma_D + e^2 D\tau\lambda^2, \tag{1}$$

where $\sigma_D \equiv ne^2\tau/m$ is the Drude conductivity. Here m, n, e, D, and τ are the electron mass, the electron density, the electric charge, the free 2DEG density of states, and the impurity-scattering lifetime, respectively. This expression has been derived for isotropic short-range potential scatterers in the Born approximation under the assumption

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that the lifetime broadening of the energy levels is smaller than the SO splitting of the band.

Numerical simulations of the longitudinal and transverse conductivities have been carried out in order to predict transport properties of Rashba 2DEG [12–16]. In numerical simulations finite size effects may importantly change the results as compared to the thermodynamic limit. In this paper we numerically compute the longitudinal conductance, its fluctuation and the localization length for isotropic and short-range scatterers and compare results with analytical predictions. The simulations enable us to explore the parameter space boundaries at which the results become independent of the system size. We believe that these results should provide guides to estimate the computational effort of numerical simulations necessary to obtain other transport properties, such as the spin Hall conductance, in the thermodynamic limit.

2. Model and method

We consider square tight-binding lattice with rectangular boundaries. In the lattice model, the Rashba Hamiltonian with short-range random potentials is given as

$$\begin{aligned} H = & \sum_{i,j,\sigma} \varepsilon_{i,j} c^{\dagger}_{i,j,\sigma} c_{i,j,\sigma} \\ & - t \sum_{i,j,\sigma} \left(c^{\dagger}_{i+1,j,\sigma} c_{i,j,\sigma} + c^{\dagger}_{i,j+1,\sigma} c_{i,j,\sigma} + H.c. \right) \\ & - \lambda_{\mathrm{SO}} \sum_{i,j,\sigma,\sigma'} \Big[- c^{\dagger}_{i+1,j,\sigma} c_{i,j,\sigma'} (i\boldsymbol{\sigma}_y)^{\sigma\sigma'} \\ & + c^{\dagger}_{i,j+1,\sigma} c_{i,j,\sigma'} (i\boldsymbol{\sigma}_x)^{\sigma\sigma'} + H.c. \Big], \end{aligned} \tag{2}$$

where the first term represents the potentials of random impurities, the second term is the hopping of electrons between nearest neighbor sites, and the last term represents the SO interaction. Site indices i and j run over all sites on the square lattice, $\boldsymbol{\sigma}_x$ and $\boldsymbol{\sigma}_y$ are the x and y components of the Pauli spin matrices. $\varepsilon_{i,j}$ takes a value V_{imp} with a probability (or concentration) c_{imp} ($0 \leqslant c_{\mathrm{imp}} \leqslant 1.0$) and zero otherwise. For small wave vectors, the second and third terms lead to the usual Rashba Hamiltonian,

$$H_0 = \begin{pmatrix} \dfrac{\hbar^2}{2m} k^2 & i\lambda\hbar k_- \\ -i\lambda\hbar k_+ & \dfrac{\hbar^2}{2m} k^2 \end{pmatrix}, \tag{3}$$

where $k_{\pm} = k_x \pm i k_y$ with $\mathbf{k} = (k_x, k_y)$, by taking $ta^2 = \hbar^2/2m$, $2\lambda_{\mathrm{SO}} a = \lambda\hbar$, and putting the band bottom of the lattice model zero. Here a is the lattice constant and is taken $a = 1$ hereafter.

In the numerical simulations, we prepare a 2D wire with a width W and a length L (the "sample") and attach semi-infinite leads on both sides (see the inset of Fig. 1). We impose the open boundary condition along the lateral direction of the system, i.e. infinite side wall barriers are assumed. The SO interaction and the random potential are non-zero only in the sample region. The conductance G in the linear response regime is calculated by using Landauer formula

$$G = \frac{e^2}{h} \mathrm{Tr}\, \mathbf{t}^{\dagger}\mathbf{t}, \tag{4}$$

where $\mathbf{t}$ is the matrix of transmission coefficients which is calculated by the recursive Green function method. The calculations are repeated for different random distributions (sampling) of the impurities from which the average of the conductance $\langle G \rangle$ and its fluctuation $\sqrt{\langle G^2 \rangle - \langle G \rangle^2}$ are obtained. The number of samples is 2000 throughout this paper.

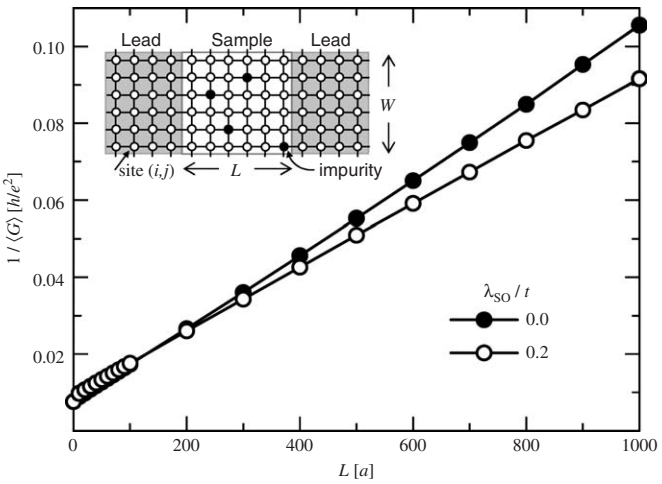

Fig. 1. Reciprocal of the configurationally averaged conductance as a function of the sample length. The wire width is $W = 200$, and the impurity potential and concentration are $V_{\mathrm{imp}} = 1.0t$ and $c_{\mathrm{imp}} = 0.1$, respectively. Results obtained in the absence and in the presence of the spin–orbit interaction are represented by • ($\lambda_{\mathrm{SO}} = 0$) and ○ ($\lambda_{\mathrm{SO}} = 0.2t$), respectively.

3. Calculated results

3.1. Conductivity

In order to deduce the electrical conductivity σ in the diffusive regime from the conductance $\langle G \rangle$ calculated for finite size cluster depicted in the inset of Fig. 1, we use the following relation,

$$\frac{1}{\langle G \rangle} = R_{\mathrm{C}} + \frac{1}{\sigma} \frac{L}{W}, \tag{5}$$

where R_{C} is a contact (Sharvin) resistance [17]. The second term represents the Ohmic resistance with well-known dependence on the geometry and material parameter σ that can be obtained from the slope of $1/\langle G \rangle$ versus L. In Fig. 1, we show the calculated $1/\langle G \rangle$ for $\lambda_{\mathrm{SO}} = 0$ and $0.2t$, and wire width $W = 200$, impurity potential $V_{\mathrm{imp}} = t$ and concentration $c_{\mathrm{imp}} = 0.1$. The Fermi level is chosen to be