Real Space Analysis of Classical Diffusion and Weak Localization of Electrons in Mesoscopic Systems from Boltzmannian Picture

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Abstract

Classical diffusion and weak localization (WL) of electrons of mesoscopic system are examined by the chaotic billiard simulation, i.e., from the Boltzmannian picture. We first present the theory and results of the analysis of WL from Boltzmannian picture applied to bulk two-dimensional electron gas (2DEG) system with the probabilistic impurity scattering. Next, we show that the squared average of the distance between the position at time t, r(t), and the initial point r(0), i.e., $\langle |\mathbf{r}(t) \cdot \mathbf{r}(0)|^2 \rangle$ is proportional to t in the mesoscopic loop array (MLA) structure for sufficiently large t. Thus, the diffusion coefficient D_{MLA} can be determined macroscopically. $D_{\rm MLA}$ values thus determined including additional probabilistic impurity scattering agreed well with the experimental values obtained from the electrical conductivity measurement at 15 mK.

1. Introduction

Recently, much attention is paid to the spin-orbit interaction (SOI) in semiconductor spintronics. Especially, the Rashba SOI [1], resulting from the structural inversion asymmetry, is important because of its gate controllability. One of the standard methods to extract the values of SOI has been the analysis of weak localization/antilocalization (WL/WAL) in 2DEG. In the WL/WAL theory, electron motions are assumed to be Brownian, not Boltzmannian, because of the mathematical convenience. However, it is more natural and transparent to consider the WL/WAL phenomena from the Boltzmannian picture, especially when considering the effect of spin precessions due to the Rashba-type SOI. This approach can be realized numerically based on the semiclassical billiard model.

The effect of WL/WAL can be expressed by the dimensionless quantity δ in the magneto-conductivity σ at sufficiently low temperatures.

$$\sigma = \sigma_0 (1 - \delta) \tag{1}$$

where σ_0 is the electric conductivity without the WL/WAL correction (denoted as "classical term"). We analyze δ and σ_0 in 2DEG and MLA, respectively, from the Boltzmannian picture in the following sections.

2. WL in 2DEG

We first show the quantitative result of the WL theory (*Brownian* picture) [2,3].

$$\delta_{\text{Brownian}} = \int_{\tau}^{\infty} dt \frac{v_F \lambda_F}{\pi} W_t \exp\left(-\frac{t}{\tau_{\phi}}\right)$$
(2)

where $\lambda_{\rm F}$ is the Fermi wave length, $v_{\rm F}$ is fermi velocity, τ is the momentum relaxation time, τ_{ϕ} is the phase coherence time and $W_t \delta S$ is the return probability within the small area δS around the origin [**r**(0)] at time *t*. The WL theory deduced the values $\delta S = dt v_{\rm F} \lambda_{\rm F} / \pi$ [m²] and $W_t = (4\pi D t)^{-1}$ [m⁻²]. We note that the concept of *return* in the Brownian picture is purely probabilistic [Fig.1(a)].

In the Boltzmannian picture, the concept of *return* is a little bit different [Fig.1(b)]. Here, we consider an ensemble of a large number of trajectories, with homogeneously distributed initial conditions, and determine statistically what portion of them have the *return count* at the trajectory length $L = v_{\rm F}t$. Then, the definition of *return* requires a predetermined "*judge length*" because the origin is just a point. For example if a particle travelling along some trajectory comes closest to the origin at the trajectory length L and the distance between this point and origin is smaller than half the *judge length*, then one obtains the *return count* one [Fig.1(b)].



Fig. 1 Schematic pictures for the concept of *return*. (a) Brownian picture. (b) Boltzmannian picture. Black point *i* in (a) and (b) shows the initial point at t=0 (origin). The blue area in (a) represents δS and the blue line in (b) shows the *judge length* for the *returning* criterion. We also show the enclosed area S in the Boltzmannian picture (b).

The conclusion of the Boltzmann picture [3, Minkov] tells us

$$\delta_{\text{Boltzmannian}} = \int_{l_{imp}}^{\infty} dL \ \frac{\lambda_F}{\pi} W_L \exp\left(-\frac{L}{L_{\phi}}\right)$$
(3)

where $W_L dL$ in unit of m⁻¹ is the ensemble average of the *return count* per unit *judge length*, l_{imp} is the mean free path in the 2DEG and $L_{\phi} = v_F \tau_{\phi}$ is the phase coherence trajectory length. The actual (physical) value of the *judge length* that gives the correct values of δ turned out to be λ_F/π . We can use Eq. (3) to calculate the weak localization effect quanti-

tatively from the Boltzmannian picture.

When the perpendicular magnetic field is applied, WL of electrons is partially broken by the magnetic field and W_L is modulated as below.

$$W_{L} = \int_{0}^{\infty} dS \ w_{\rm cl}(S,L) \cos\left(2\pi \frac{BS}{h/2e}\right) \tag{4}$$

where $w_{cl}(S, L)dS$ is portion of W_L which has the encircling (enclosing) area (absolute value) between *S* and *S*+*dS*. The cosine term represents the effect of the magnetic field on the quantum interference between the time-reversal pair of the classical trajectories of electrons [4].

In the Browniann picture, the function $w_{cl}(S, L)$ can be obtained by the Wiener measure of the diffusion equation. In this work, we obtain $w_{cl}(S, L)$ from the Boltzman picture numerically. We then compare the obtained results with the existing well-known WL/WAL theories [5].

3. Classical Diffusion in MLA

Next, we investigate the classical diffusion in the mesoscopic loop array (MLA) structure from the Boltzmannian picture. The particular structure of our MLA is shown in Fig. 2. The electric conductivity (classic term) in MLA, $\sigma_{\rm MLA}$, is related to the diffusion coefficient $D_{\rm MLA}$ by Einstein's relation as below.

$$\sigma_{\rm MLA} = e^2 \rho_{\rm MLA} D_{\rm MLA} \tag{5}$$

Here the density of states ρ_{MLA} is related to the 2DEG bulk value $m^*/\pi\hbar^2$, but reduced by 0.524, which is the portion of the conductive part in MLA out of the whole sample area that contributes to the electric conductance. D_{MLA} can be defined as $\langle |\mathbf{r}(t)-\mathbf{r}(0)|^2 \rangle/4t$ if the mean squared distance $\langle |\mathbf{r}(t)-\mathbf{r}(0)|^2 \rangle$ is proportional to *t* for sufficiently large *t*. We apply the chaotic billiard simulation (Boltzmannian picture) to calculate $\langle |\mathbf{r}(t)-\mathbf{r}(0)|^2 \rangle$ numerically. D_{MLA} can also be calculated by velocity-velocity correlation $D_{\text{MLA}} = 0.5 \times$ $\int \langle \mathbf{v}(t) \cdot \mathbf{v}(0) \rangle dt$, which is mathematically equivalent to $\langle |\mathbf{r}(t)-\mathbf{r}(0)|^2 \rangle/4t$.

Fig. 3 (a) shows the snapshots of the classical diffusion of the particles placed in the black ring at the center at t = 0using the Boltzmannian picture (15,232 initial conditions), where $L = v_F t$ and the probabilistic impurity scattering with $l_{imp} = 1.0 \ \mu m$ is also included. We found that the mean squared distances $\langle |\mathbf{r}(t)-\mathbf{r}(0)|^2 \rangle$ are 4.48, 40.26 and 399.28 μm^2 for L = 10, 100 and 1000 μm , respectively. Therefore, the time (length) scale where $\langle |\mathbf{r}(t)-\mathbf{r}(0)|^2 \rangle$ becomes proportional to t (or L) is approximately $t > 1.18 \times 10^{-10} \text{ sec } (L >$ 100 μm). The D_{MLA} value thus deduced is $8.5 \times 10^{-2} \text{ m}^2/\text{s}$.

In Fig. 3 (b), we show the calculated values D_{MLA} as a function of the the probabilistic mean free path l_{imp} . This can be compared to the experimental values in Fig. 3 (c), which were obtained from the experimental electric conductivity values at 15 mK and using Eq. (5). From these results, the l_{imp} values in the experimental system turned out to be in the sub-micrometer order ($l_{\text{imp}} < 1 \ \mu\text{m}$), which agrees with the preliminary results obtained from the quantum mechanical analysis of WL/WAL correction δ in Eq.

(1) in this MLA system.



Fig. 2 Schematic diagram for the Hall bar sample used in the present work. The left and right panels show the SEM micrograph and the Hall bar device of MLA, made of InGaAs/InAlAs quantum well, used in the measurement. We have 5,408 rings in the actual Hall bar.



Fig. 3 (a) Snapshots of classical diffusion of Boltzmannian electrons in MLA with $l_{imp} = 1.0 \ \mu m$. (b) The D_{MLA} values by the chaotic billiard simulation as a function of l_{imp} . Here, we use $v_F = 8.51 \times 10^5 \text{ m/s.}$ (c) The experimental values of D_{MLA} as a function of V_g .

3. Conclusions

In this work, we illustrate the probabilistic and statistical features of the weak localization in the bulk 2DEG system from the Brownian and Boltzmannian pictures, respectively. We also calculated the classical diffusion coefficient $D_{\rm MLA}$ in a specific MLA structure using the Boltzmannian picture. The obtained $D_{\rm MLA}$ values agreed with the experimental results deduced from the electric conductivity measurements at 15 mK. We therefore conclude that the electric conduction in the MLA system can be understood from the viewpoint of the diffusion of Boltzmaniann particles. **References**

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